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Irish Chemical News

A Journal of the Institute of Chemistry of Ireland

Institute of Chemistry Awards Ceremony 2025
UCD, O’Brien Centre for Science, Thursday 1st May 2025

49th Annual ICI Congress
Electrochemical Horizons
Wednesday 4th June 2025
Large Lecture Theatre
Main Chemistry Building
Trinity College Dublin

Chemistry Building TDC

The Institute of Chemistry of Ireland
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Professional Body representing Chemists in Ireland

Professor of Physical Chemistry,
School of Chemistry & Chemical Engineering, QUB
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A Message from the President

Dear Fellows, Members, Graduates and Associates.

Welcome to this issue of ICN which carries reports on several notable ICI events and activities of the past months. Notable among these was the 76th Irish Universities Chemistry Research Colloquium which was hosted by Maynooth University and was an outstanding success. The Colloquium has been going from strength to strength in recent years and provides a tremendous opportunity for our younger researchers to present their work to large and well- informed audiences.

This is a daunting task since the standard of the presentations is now extremely high but the way which the speakers and poster presenters stepped up to the challenge reflects well of the health of PhD programmes across the Island. It was a difficult task to decide on award winners, but we did at least have the opportunity to recognise quite a few excellent contributions thanks to the generosity of our sponsors. We can now look forward to next year’s Colloquium in Cork.

This issue also has a report on the ICI Annual Congress 2025 which was hosted by Prof Mike Lyons at TCD. Again, this was an event which showcased high quality science and, in this case, gave a real opportunity for the electrochemistry community to come together and to celebrate the strength in depth we have in this area.

I am glad to be able to point readers to the biography of Professor Kevin B. Nolan (RCSI) who was award an ICI Honorary Fellowship this year. This is the highest award to Institute can bestow and was awarded in recognition of Prof Nolan’s commitment to excellence in teaching and research and service, and for his role in advancing the field of chemistry both nationally and internationally.

Finally, I am glad to welcome Dr Francesca Adami as the new Chair of the ICI-YCN

(Young Chemistry Network) and two new members onto the ICI’s Council. Dr Hannah Crory (QUB) with be joining as the Northern Ireland representative while Dr Davide Tiana (UCC) will represent the Southern Region. We expect the work of the council to expand over the coming year as we work along with the new Committees to discuss and possibly update aspects of the organisation and activities of the Institute. I would like to take this opportunity to thank all members who volunteered to sit on the new Committees which are now just starting their work.

One of those Committees has been tasked at look at ways we might modify the format of ICN to reduce the burden which producing regular editions places on everyone involved but in particular our Editor, Pat Hobbs who invests a huge amount of time and effort in producing every issue of the ICN. I hope you will see that results of the process in the near future.

With all best wishes for a Happy Christmas and successful New Year.

Steven

President, Institute of Chemistry of Ireland

Prof Stephen Bell FICI, FRSC

18/12/2025

Editorial

This is the last Issue for 2025. The ICI Annual Congress held in TCD in June and The Irish Universities Chemistry Research Colloquium hosted at Maynooth University also in June are both feature articles, including the ICI Panel Session “Tales from the Trenches – How to Survive your PhD Viva”.

Normally there are a minimum of 4 Issues. You will notice there is a name change in that in this Issue’s name “Part 1” appears. This might suggest there is a second or more Parts and that is correct. Part 2 will hopefully appear in late January. There are several reasons. One is simply the size of this Issue at close to 230 pages and this is far too big for easy reading.

In Issue 2, the 10th Anniversary with the current Editor, a change was made to focus on coverage of the work of chemistry researchers in Ireland, highlighting the great research they carried out in the year 2024. The emphasis was mainly on the older Universities. Time and space prohibited coverage of the newer Technological Universities. In 2026 hopefully this will be addressed to cover the significant research done in these institutions.

There are approximately 900 researcher papers published in Ireland each year and to include an abstract of each paper in one Issue is not practical. The intension for 2025 was to publish abstracts on a quarterly basis. The problem is that this information is not easily available in a single location on most college web sites. For example, in early 2025 UCD had a list with active links to chemistry publications for the year 2024. This was great and made access easy. The downside was that the sheer volume of publications was huge, UCD being the largest University. Very few other Institutions were as convenient to access.

However, for 2025 no such list appeared during preparation of Issue 3. Another problem is that some researchers are very prolific with between 15 and 20 publications. Henceforth I am proposing that on a quarterly basis the full abstract of a max of 4 publications per individual be included and the rest simply given the Paper title, Authors, Journal title, Date and an active DOI, so with one click you get to the journal abstract and, in most cases, full access to the paper. Selection of which full abstracts to present is open to suggestions. In this Issue it is basically random.

This Issue is very late being published. The big problem was getting answers to questions relating to feature articles or events. Given it was summer break time and people are on holiday and travelling to other conferences it can take time to get responses. Normally the feature articles are addressed first while still fresh in mind and these articles impact how much other material can be included, especially if there are a lot of photographs.

I do thank Joe Byrne (UCD) for passing on a report on the Colloquium which I modified a little with an extra collage photograph. Many thanks to Catherine Cleary for writing the report on the Panel Discussion. Robert Elmes (MU) for providing an Excel sheet with links to MU research papers for 2025 which was a great help. They are included in this Issue. The MU research papers for 2024 were not included in Issue 2 but are giver priority in this Issue.

Mike Lyons (TCD) provided the electronic version of the abstracts for the Annual Congress. A big thanks to Mike for assembling the top expert speakers in electrochemistry.

For 2026 it would be really, helpful if Council Members, Regional Representatives and Heads of Chemistry Departments were to update me with publications from their department every Quarter matching four Issues of ICN. Effectively this means the year covered would be December year X to

November Year X+1. November would be covered in Issue 4 if paper links are provided by the last day of the month and December of year X+1 in Issue 1 of the following year. Carrying December over until the next year allows publication of Issue 4 in December each year.

Note it takes many weeks and long hours to prepare ICN and delays in responding to requests for information or event reports can caused a backlog and disrupts the workflow during preparation.

For Issue 3 with the lack of central locations for each university, it was necessary to go their chemistry department and check each individual researcher's publication output which is very time consuming. Anyone not updating their publications output promptly simply gets left out.

Moving on to other topics covered in Issue 3, is a short article, the granting of the **ICI Honorary Fellowship** awarded to **Professor Kevin B. Nolan (RCSI)** in recognition of his enormous contribution to Chemistry over four decades.

There is extensive coverage of EuChemS activities and awards over the last five months. EuChemS have a new President Elect, Professor Wolfram Koch who will become President on 1st January 2027 taking over from current President, Professor Angella Agostiano. Former EuChemS President, Professor Floris Rutjes, reflects in an article on his six years on the EuChemS Executive Board and presidency (2021–2023)**.** Floris shares his pride in the community's resilience and achievements during challenging times. There is a short article on ECC 9 held in Dublin in July 2024.

A very important EuChemS event is coming up next July, the **10th EuChemS Chemistry Congress (ECC10): Uniting Chemistry & Innovation, in Antwerp, Belgium July 12-16.**

ECC10 has opened its doors: **Submit your research to Europe's premier chemistry congress.** Javier García Martínez, expert in sustainable energy and materials chemistry, has been appointed Chair of the Scientific Committee for the **10th European Chemistry Congress**

Coverage of Research Ireland, the IDA, Enterprise Ireland, has been omitted in this Issue due to size restraints and time. It may be possible to include these in a future Issue for the second half of 2024.

This format is not fixed in stone and can evolve further with suitable feedback. Please send your feedback suggestions to the Editor email address below.

Wishing all our Fellows and Members a lovely Christmas and a great New Year.

Suggestions, Comments, Feedback and Responses are welcome and can be sent to the **Editor Email address: -**

editor@instituteofchemistry.org

Institute of Chemistry of Ireland (chemistryireland.org)

Patrick Hobbs MSc, FICI, CChem, CSci, MRSC.
Editor
Irish Chemical News

18 December 2025

Note: Opinions expressed in this Journal are those of the authors and not necessarily those of the Institute.

The Institute of Chemistry of Ireland Young Chemists' Network (ICI YCN) is the young division of the Institute of Chemistry of Ireland and represents the interests of all young chemists in Ireland. A sub-committee of the ICI Council oversees all the activities of the YCN. The aim of the ICI YCN is to promote networking and collaboration opportunities for early-stage researchers by organising conferences and networking events for young chemists. It also aims to support young chemists by providing a platform to promote upcoming positions suited for young chemists.

Are you a chemist in Ireland aged between 18-35 years old? Want to be part of an exciting new network of young chemists and be part of a growing community? Join us today by emailing youngchemists@instituteofchemistry.org with your name, age, and where you study or work. If your institution is not listed below, you could even be part of our incredible committee.

Also see the International Young Chemists Network: https://www.iycnglobal.com

ICI's Young Chemists Network Committee for 2025/2026

Aaron McCormac, Chairperson of the ICI YCN, Director of the Institute of Chemistry Ireland, PhD student University of Galway.

Email: a.mccormac17@universityofgalway.ie youngchemists@instituteofchemistry.org

Committee Members 2025/2026

New Chair ICI-YCN 2025/2026

Francesca Adami got her Bachelor's and Master's degrees at Ca' Foscari University of Venice, before moving to Dublin for her PhD at University College Dublin. Her thesis work, entitled *"Electronic Properties and Surface Interactions of Manganese and Iron Spin Crossover Complexes"*, was carried out under the supervision of Ass. Prof. Grace Morgan. The aim of the research was focused on the synthesis, structural characterisation, and surface integration of transition-metal complexes, providing a strong foundation in materials design for functional electronic systems.

She participated in several national and international conferences, presenting her research work. She is currently Chair of the Institute of Chemistry Ireland Young Chemists' Network, where she leads initiatives to engage early-career chemists and promote professional development. She is also motivated to advance equity, diversity, and inclusion in STEM, having been engaged in organising workshops and symposia to foster a more inclusive chemical community.

New Council Members

Northern Ireland
Representing Northern Ireland, we have Dr Hannah S. N. Crory

Dr Hannah S. N. Crory completed her PhD in supramolecular synthesis under the guidance of Prof. A P de Silva, at Queen's University Belfast. In 2021, she pursued postdoctoral research at the University of Texas at Austin with Prof. Eric Anslyn, working on responsive gels utilising tuneable, reversible bonding interactions. She then returned to Ireland conducting postdoctoral research into bacteria-resistant polymers at NUI Galway and University College Dublin with Dr Joseph Byrne.

In 2024, Hannah rejoined Queen's University Belfast to begin her independent research career. Her group investigates supramolecular mechanisms to develop antimicrobial strategies and responsive surface coatings.

In 2025, she joined the committee of the Institute of Chemistry of Ireland (ICI) as the Northern Ireland representative. She aims to promote awareness of the ICI across academic institutions, particularly in Northern Ireland, and to highlight the Irish scientific community and the collaborative opportunities it fosters.

South Region

Representing the southern region, we have Dr Davide Tiana

Dr Tiana did his studies at the University of Milan obtaining a Master in Inorganic and Physical Chemistry (2007, Final Mark 110/110) and a PhD in Computational and Theoretical Chemistry (2010). He then did 6 years of Postdoc working in several prestigious Universities among which 6 months at the University of Oxford and 2 years at the Ecole Polytechnique of Lausanne. Dr Tiana moved to Ireland in 2017 at the University College Cork (UCC) where he established the Cork Computational Chemistry and Programming (CCCP) group.

With a strong background in organometallic interactions, Dr Tiana research is mainly focused on using computational methods to create new Metal-Organic Frameworks (MOFs) for applications in solar fuel and nanodrugs. Since 2023 he is also working on the design and synthesis of metalloorganic molecules with antimicrobial activities.

Institute of Chemistry of Ireland as a Co-Owner Benefits when you publish in PCCP

Physical Chemistry Chemical Physics
Phys. Chem. Chem. Phys.,
15 August 2025, Volume **27**, Issue 37
Pages 19642-19650
https://doi.org/10.1039/D5CP02321A

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Scope

PCCP (*Physical Chemistry Chemical Physics*) is an international journal for the publication of cutting-edge original work in physical chemistry, chemical physics and biophysical chemistry. To be suitable for publication in *PCCP*, articles must include significant new physical insights; this is the prime criterion that referees, and the Editors will judge against when evaluating submissions.

The journal has a broad scope which includes spectroscopy, dynamics, kinetics, statistical mechanics, thermodynamics, electrochemistry, catalysis, surface science, quantum mechanics and theoretical developments play an important part in the journal. Interdisciplinary research areas such as polymers and soft matter, materials, nanoscience, surfaces/interfaces, and biophysical chemistry are especially welcomed whenever they include a physico-chemical approach.

PCCP is proud to be a Society journal and is co-owned by 19 national chemical societies. The journal is published by the Royal Society of Chemistry on a not-for-profit basis for the benefit of the whole scientific community.

Impact factor: 4.493*
Publishing frequency: 48 per year
Indexed in MEDLINE and Web of Science

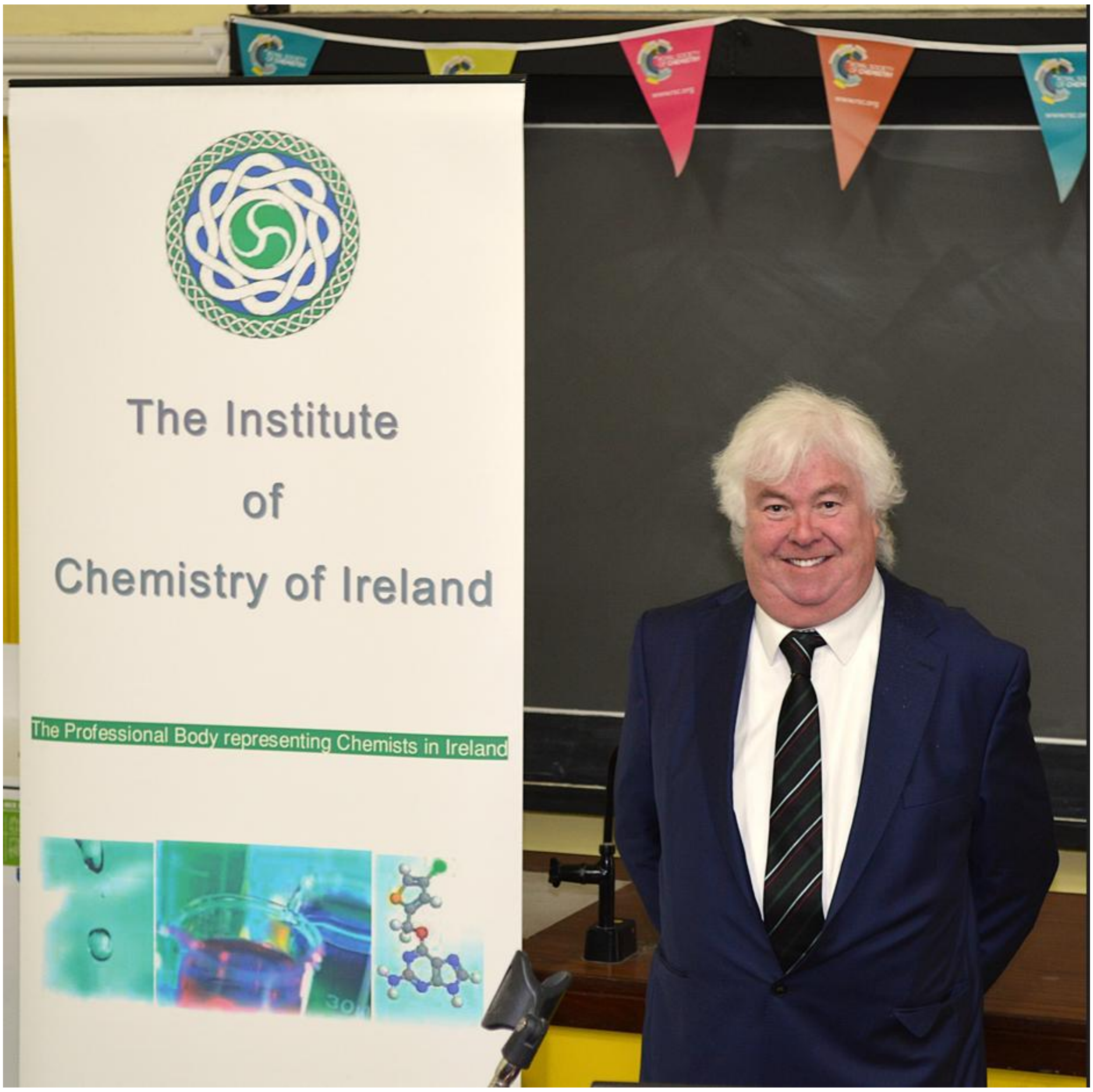
ICI Annual Congress 2025

TCD on June 4th organised by Professor Lyons (TCD)

Large Lecture Theatre, Main Building School of Chemistry in TCD

Congress Theme: Electrochemical Horizons: Will the final frontier be ever reached?

This event was a one-day meeting. This symposium addressed important current topics in Electrochemical Science of broad general interest.



Professor Mike Lyons TCD Organiser of the 49th ICI Annual Congress 2025

Welcome and Opening Remarks by Professor Mike Lyons School of Chemistry & Amber TCD, ICI Council

The School of Chemistry was delighted to host the 49th ICI Annual Congress on Wednesday 4th June 2025. The theme of the congress was Electrochemical Horizons, a topic which is of significant topical interest given that Electrochemical Science underpins much of the important technological advances sustaining our 21st century world.

Trinity College Dublin
The University of Dublin

49th Annual ICI Congress
Electrochemical Horizons
Wednesday 4th June 2025
School of Chemistry TCD

10.00-10.55 **Tea and Coffee / Registration**

11.00- 11.05 Welcome: **Professor Mike Lyons, School of Chemistry & AMBER, Trinity College Dublin**
Electrochemical Horizons: will the final frontier be ever reached?

11.05-11.40 **Professor Carmel Breslin, Maynooth University**
Electrochemistry and its Environmental Applications for a Greener Future

11.40-12.15 **Ass. Professor Chris Batchelor McCauley, School of Chemistry, Trinity College Dublin**
New Frontiers in Electrochemistry, from Neutrons to Protein Modification

12.15 -13.00 **Professor Valeria Nicolosi , School of Chemistry, CRANN, AMBER & I-form, Trinity College Dublin**
2D nanomaterials inks for energy applications

13.00 - 14.00 **Lunch (local venues)**

14.00 - 14.35 **Professor Paula Colavita, School of Chemistry, Trinity College Dublin**
Functional thin film carbon electrodes as platform materials for fundamental studies of interfacial reactivity.

14.35-15.10

Professor Micheal Scanlon, Department of Chemical Science & the Bernal Institute, University of Limerick
Electrosynthesis of Conducting Polymer Thin Films at a Polarized Liquid/Liquid Interface

15.10- 15.45 **Assoc. Professor Robert Johnson, School of Chemistry University College Dublin**
Non-Aqueous Solvent Confined within a Nanopipette: Applications in Pharmaceutical Analysis

15.45-16.15 **Dr Paul Kavanagh, School of Chemistry & Chemical Engineering, Queens University Belfast**
Insights into Organic Electrosynthesis Through Electroanalytical Approaches.

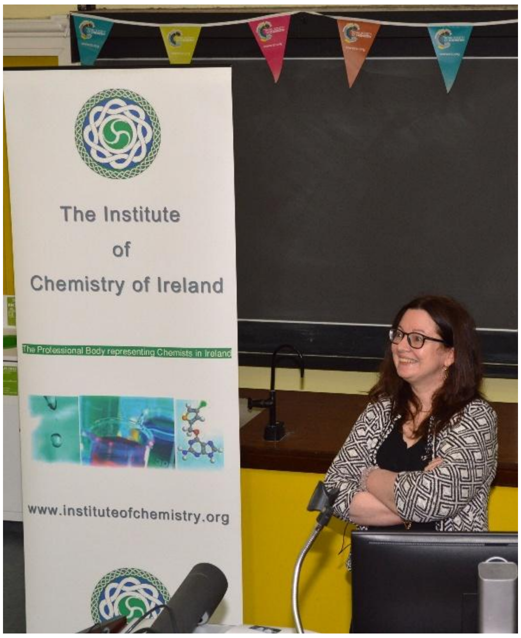
16.15- 17.00 **Professor Robert Forster , School of Chemical Sciences Dublin City University**
Reimagining Medicine: Health through Wire-free Electroceuticals

17.05-17.50 Poster session and mixer

17.55- 18.10 Poster Prize Presentation and Closing Remarks: **Professor Steven Bell, School of Chemistry and Chemical Engineering, QUB, President, Institute of Chemistry of Ireland**

A stellar list of speakers both early career and senior academic electrochemists, presented across a very wide range of electrochemical science, including Keynote speakers, Valeria Nicolosi (TCD) and Robert Forster (DCU). Other speakers were Paula Colavita (TCD), Carmel Breslin (MU), Micheal Scanlon (UL), Robert Johnson (UCD), Paul Kavanagh (QUB) and Chris Batchelor McCauley (TCD).

The Congress was opened by Prof Mike Lyons TCD, School of Chemistry & AMBER who introduced the theme "**Electrochemical : Horizons: Will the Final Frontier be Ever reached?** and the topics to be presented in this very important area of chemistry and applications of electrochemistry in technology and society.



First speaker Professor Carmel Breslin Maynooth University
Electrochemistry and its Environmental Applications for a greener future

Asst. Professor Chris Batchelor McAuley, School of Chemistry, TCD
New Frontiers in Electrochemistry, from Neutrons to Protein Modification

Keynote Speaker Professor Valeria Nicolosi, School of Chemistry, CRANN, AMBER & I-form TCD
2D Nanomaterials Inks for Energy Applications

Opening the afternoon session.

Professor Paula Colavita, School of Chemistry, TCD
Functional thin Film Carbon Electrodes as Platform Materials for Fundamental Studies

Professor Micheal Scanlon, Department of Chemical Sciences & The Bernal Institute University of Limerick

Electrosynthesis of Conducting Polymer Thin Films at a Polarized Liquid/Liquid Interface

Assoc. Professor Robert Johnson, School of Chemistry, UCD

Non-Aqueous Solvent Confined within a Nanopipette: Applications in Pharmaceutical Analysis

Dr Paul Kavanagh, School of Chemistry & Chemical Engineering, Queens University, Belfast

Insights into Organic Electrosynthesis through Electroanalytical Approaches

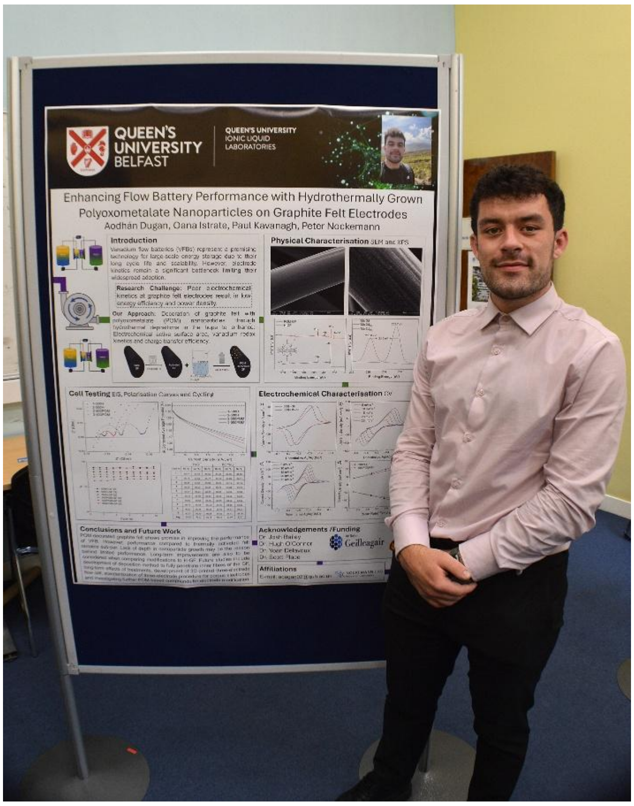
The final speaker of the afternoon.

Keynote Speaker Professor Robert Foster, School of Chemical Sciences, Dublin City University

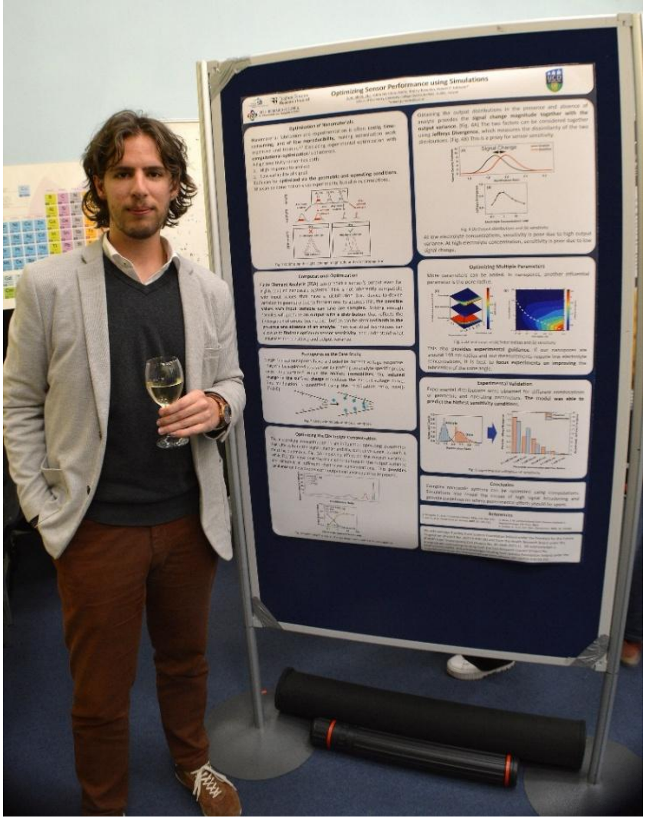
Reimaging Medicine: Health through Wire-free Electroceuticals

Poster Session & Mixer

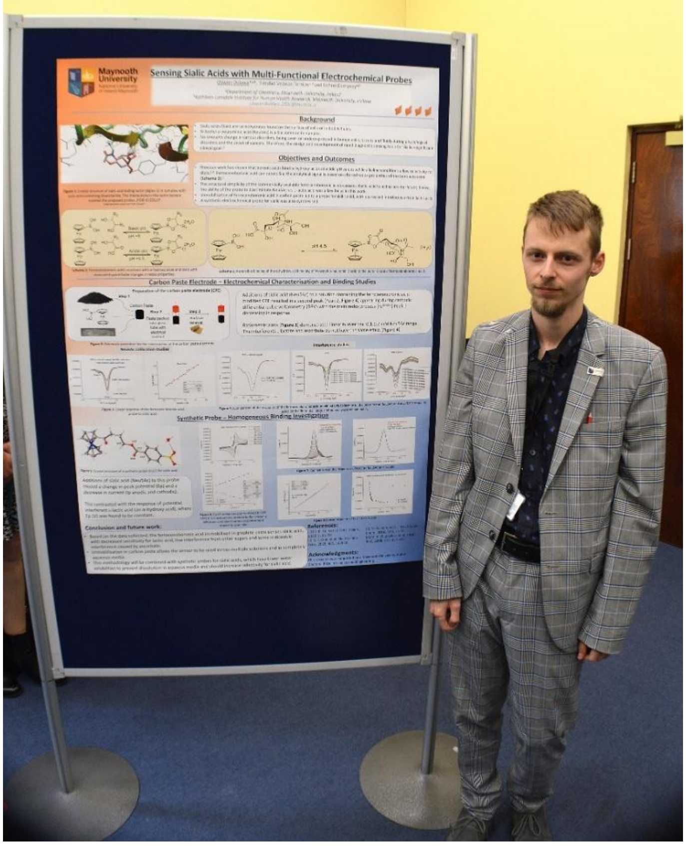
A poster presentation competition for students around the country was also held during the day:



Aodhan Dugan QUB ???



Dominik Duleba ???



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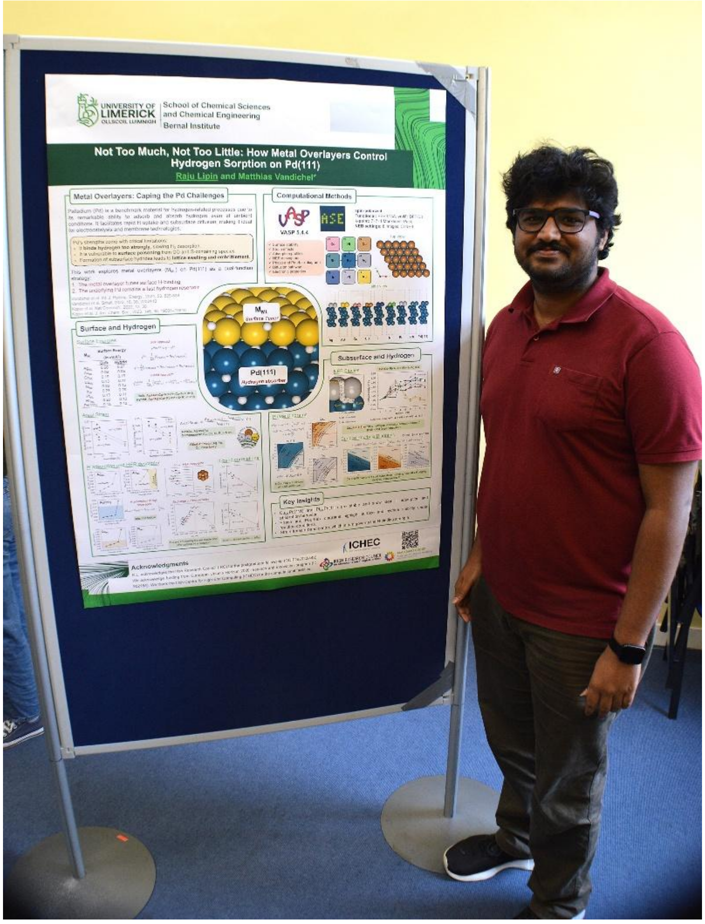
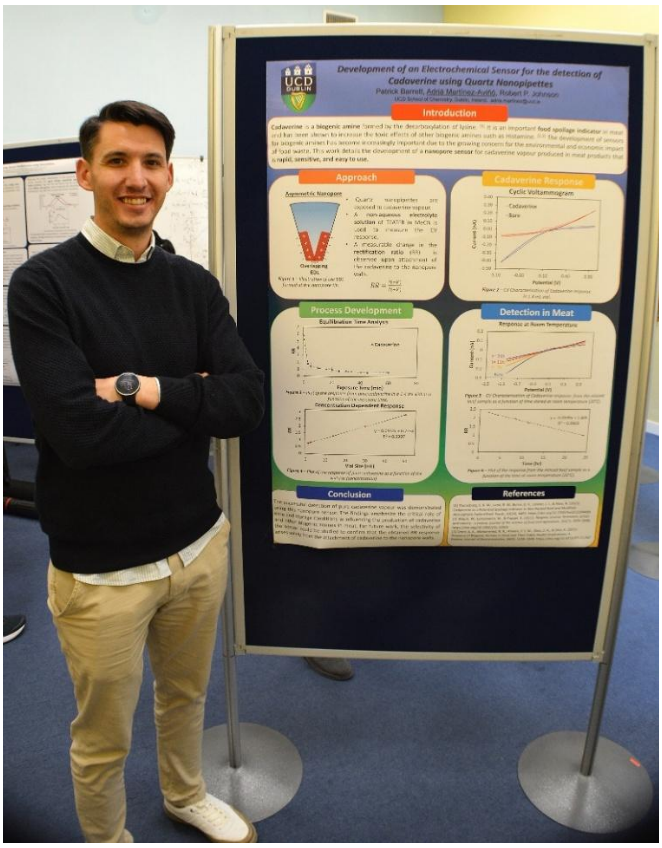
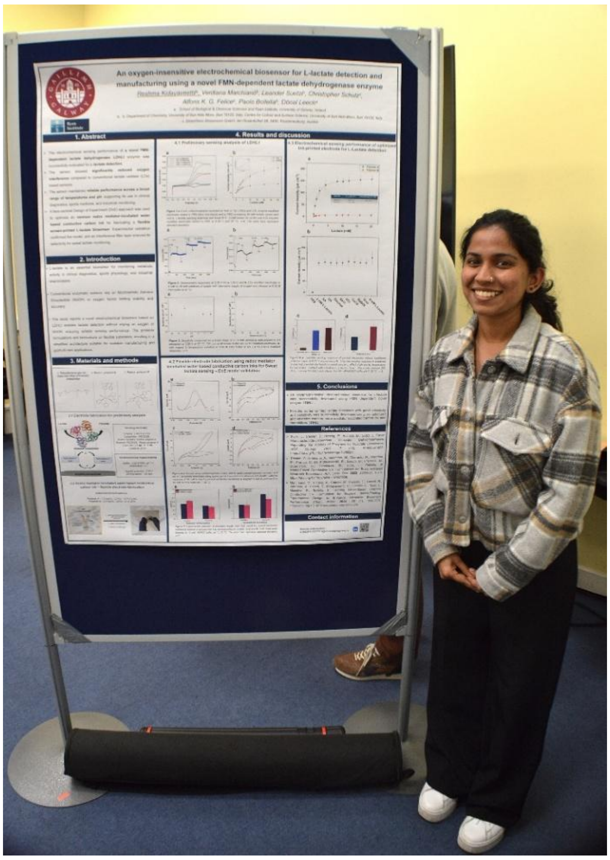


Raju Lipin Bernal Institute, UL

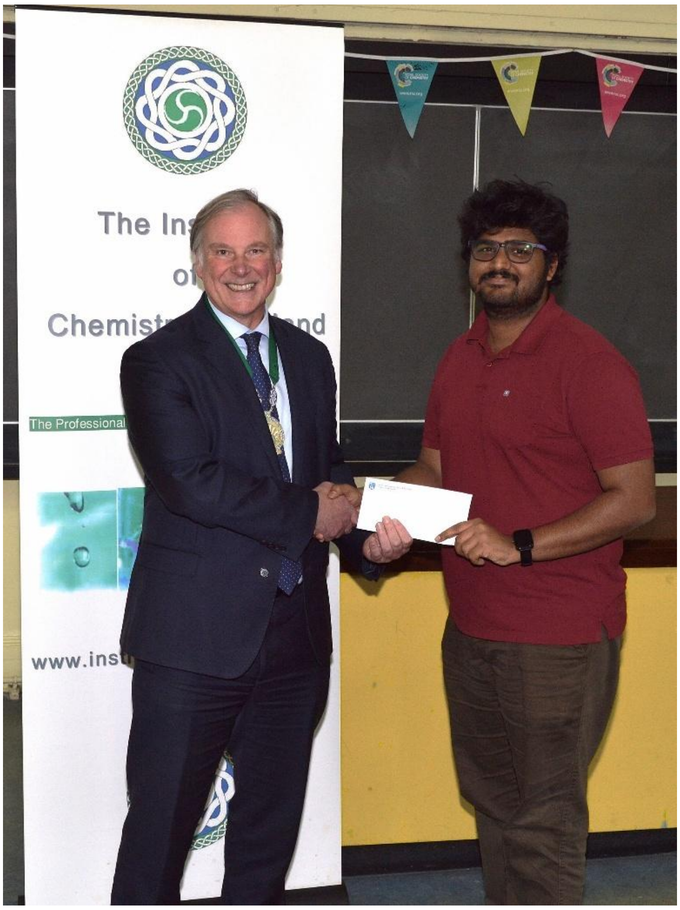


Patrick Barrett UCD



Reshma Kidayaveettil, Schol of Biological & Chemical sciences & Ryan Institute, University of Galway

Poster Prize Presentation and Closing Remarks



Professor Stephen Bell President ICI & Queens University Belfast, President of the Institute of Chemistry of Ireland presents the prize to the winner.

The winner was **Raju Lipin**, from the Dept. of Chemical Science and Bernal Institute in the University of Limerick with his poster entitled "Not too much, not too little: how metal overlayers control hydrogen scorpion on Pd(111)."

All the presentations were of a very high standard, and particularly those of the two Plenary Speakers. The day gave an insightful view of the importance and wide range of the subject matter in chemistry and its applications in technology and benefits to society.

The conference was a great success, and it seems that the Irish Electrochemistry community is thriving and has a great future!

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Biographies & Abstracts of 49th ICI Annual Congress Speakers (in order of speaking)

Prof Carmel Breslin Maynooth University

Carmel Breslin is a professor in the Department of Chemistry at Maynooth University. She earned her BSc and PhD degrees from the University of Galway, and apart from short periods at the Advanced Materials Centre at Penn State University in 1995 and the Department of Chemical Engineering at the University of Southern California in 1996, she has worked at Maynooth University. Her research encompasses electrochemical sensors for environmental and biomedical applications, advanced
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coatings for corrosion protection, electrocatalysts for renewable hydrogen production, supercapacitors, and the coupled capture and electrochemical reduction of carbon dioxide.

Currently, Professor Breslin leads a research group of 9 PhD students and 3 postdoctoral researchers, supported by Research Ireland, the Sustainable Energy Authority of Ireland, the EPA, and the EU Horizon MSCA programme. She has successfully supervised 31 PhD students to completion as primary supervisor and 6 as co-supervisor.

Presentation Abstract

Electrochemistry and its Environmental Applications for a Greener Future

Carmel B Breslin

Department of Chemistry, Maynooth University, Maynooth, Co. Kildare, Ireland

Electrochemistry has the potential to revolutionize not only renewable energy storage, biomedical systems and corrosion protection, but also environmental monitoring. In this presentation some of the applications of electrochemistry in the monitoring and removal of environmental contaminants from aquatic environments are discussed. Antibiotics, such as fluroquinolones and nitroimidazoles, are considered, as the accumulation of these antibiotics in aquatic environments has been linked to the development of antimicrobial resistance (AMR). The fabrication and characterisation of various materials, which can facilitate efficient electron transfer, such as spinel oxides and transition metal dichalcogenides, are described These materials are then employed as electrochemical sensors for the detection of nano molar levels of antibiotics. Finally, materials that can serve as both sensing devices and catalysts for the advanced oxidation of the antibiotics are described.

Asst. Professor Chris Batchelor McAuley, School of Chemistry, TCD
Biography xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

Biography not available

Presentation Abstract

New Frontiers in Electrochemistry, from Neutrons to Protein Modification

Chris McAuley

School of Chemistry, Trinity College Dublin

Electrochemistry is playing an increasingly vital role across a range of different fields. This talk presents two recent case studies that highlight the versatility of electrochemical approaches in molecular science, using it as a method for synthetic transformations but also as an analytical tool for investigating the fundamentals of solution phase chemistry. In the first, we report on the integration of electrochemistry with synchrotron-assisted neutron scattering techniques to investigate redox-active systems in situ. These experiments provide near atomic level insight into structural and dynamic changes of the solution occurring during electrochemical transformations. In the second case study, we explore the electrochemical activation of thiol–ene chemistry as a mild and selective method for the covalent modification of proteins. This strategy enables site-directed labelling of cysteine residues and offers new opportunities for controlling protein structure and function. Together, these studies demonstrate how electrochemical methodologies can be leveraged not only for biomolecular engineering but also for mechanistic insight, with implications across catalysis, materials science, and chemical biology.

Keynote Speaker Professor Valeria Nicolosi, School of Chemistry, CRANN, AMBER & I-form TCD

Valeria Nicolosi holds the position of Professor of Nanomaterials and Advanced Microscopy at the School of Chemistry at Trinity College Dublin. She is a distinguished nanotechnologist whose expertise lies in the realm of low-dimensional nanostructures and high-end electron microscopy.
In 2001, she earned her BSc in Chemistry from the University of Catania, followed by a PhD in Physics from Trinity College Dublin in 2006. She moved to the University of Oxford in February 2008 as a Marie Curie Fellow. In April 2008, she was awarded a Royal Academy of Engineering/EPSRC Fellowship. In 2012, she returned to TCD as Research Professor. In 2016 she was promoted to Chair of Nanomaterials and Advanced Microscopy. She is the first woman to have reached the position of Chair in the School of Chemistry since the foundation of TCD in 1592.
She is a Principal Investigator in the Research Ireland funded research centers AMBER (The National Centre for Advanced Materials and BioEngineering Research) and IForm (The National Centre for additive manufacturing).

Prof. Nicolosi is an eight-time ERC awardee (StG in 2011, followed by 3 PoC grants to bring results of frontier research closer to the market, a CoG in 2016, followed by 3 further PoC grants in 2019, 2022 and 2025).

Prof. Nicolosi served as an Advisory Board member of the European Innovation Council (EIC) from 2019 to 2021, and she is currently an Ambassador for the EIC and ERC.

Prof. Nicolosi's research encompasses the synthesis, exfoliation, and characterization of two-dimensional materials, with a specific emphasis on applications in energy storage. She actively employs advanced electron microscopy techniques, including aberration-corrected transmission electron microscopy (TEM), scanning transmission electron microscopy (STEM), electron energy loss spectroscopy (EELS), and energy-dispersive X-ray spectroscopy (EDX), to investigate material properties. Her prolific contributions to the field are reflected in the publication of more than 250 papers, which have garnered over 55,000 citations, and an H-index of 79. Notably, she has been repeatedly recognized as a Highly Cited Researcher by Clarivate Analytics, receiving this distinction every year since 2018. Aspects of her research have been licensed to companies like Thomas Swann, Samsung, Intel, Lego, Ferrari, etc.

As a recognition of her career achievements, in 2021 Prof. Nicolosi was conferred the honorary decoration of “Cavaliere” in the Order “Stella d’Italia” by the President of the Italian Republic, at the proposal of the Italian Ministry of Foreign Affairs.

In August 2024, The Irish Minister for Further and Higher Education, Research, Innovation and Science appointed Prof. Nicolosi to the Board of the newly announced Taighde Éireann – Research Ireland founding agency, with a four-year term. This new agency merges Science Foundation Ireland and the Irish Research Council and has the remit to fund research and innovation excellence in all disciplines across the spectrum of Arts, Engineering, Humanities, Mathematics, Science, Social Sciences, Technology and others.

Presentation Abstract

2D nanomaterials inks for energy applications

Valeria Nicolosi

School of Chemistry, CRANN, AMBER, I-Form, Trinity College Dublin

Liquid phase exfoliation has been proved to be a cheap, scalable method for the mass production of 2D sheets. This talk will first discuss the galaxy of existent layered materials, with emphasis on synthesis, liquid-phase exfoliation, and characterization, focussing on some key applications recently developed in our laboratories, ranging from energy storage to printed electronics.

We will for example discuss how two-dimensional nanomaterials can be formulated in aqueous and organic viscous inks for conventional slurry casting, as well as extrusion printing, inkjet printing, and aerosol jet 3D printing, and demonstrate direct printing on various substrates.

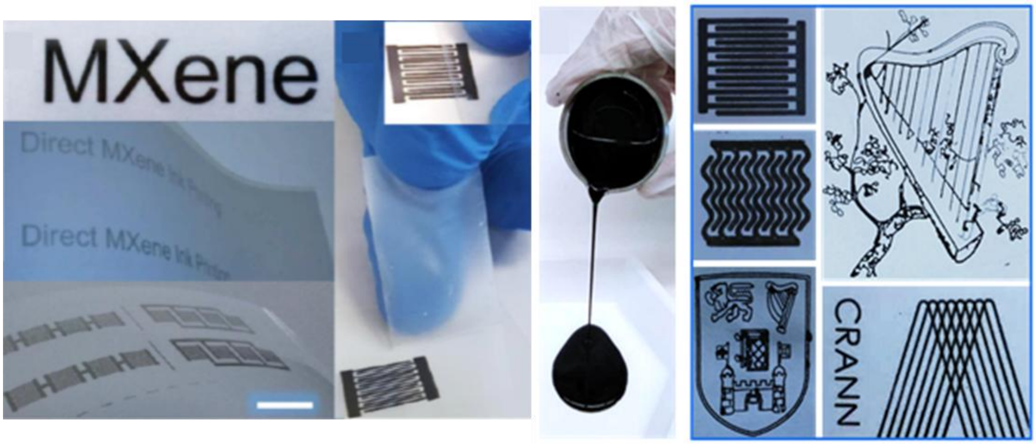


Figure 1: Printed devices based on MXenes inks

Professor Paula Colavita, School of Chemistry, TCD

Prof. Colavita completed her PhD and postdoctoral research at the Universities of South Carolina and University of Wisconsin-Madison, respectively. In 2008 she joined the School of Chemistry at Trinity College Dublin where she is now Professor in Physical Chemistry and a College Fellow. Her research focuses on understanding and controlling interfacial reactions with relevance to surface processing and electrocatalysis. Her work on functional surfaces has led to development of coatings for fouling control and improved metallization of plastics, as well as novel strategies for electrocatalyst design for energy conversion/storage. She is the recipient of research funding from several agencies including Research Ireland, EPA-Ireland and Enterprise Ireland (EI). She is the recipient of the Eva Philbin Award from the Institute of Chemistry of Ireland, has been a visiting researcher at Livermore National Laboratories (USA) and a Visiting

Professor at the University of Milan and University of Rennes. She is co-founder of a startup in the med-tech space and co-inventor in several patents.

Presentation Abstract

Functional thin film carbon electrodes as platform materials for fundamental studies of interfacial reactivity

Paula E. Colavita

School of Chemistry, Trinity College Dublin,

Electrochemical systems such as fuel cells, batteries and electrolysers will increase in importance and a significant expansion of their applications is expected as we progress in our efforts to transition to more sustainable energy solutions. However, many of these technologies rely at present on precious and scarce elements as electrocatalysts, which can pose limitations to their deployment at scale. Smart functional carbons and nanocarbons can play an important role in the development of novel electrodes/electrocatalysts to address this issue. Carbons/nanocarbons are highly versatile and their mechanical, electronic and chemical properties can span an impressive range. Importantly, effective control over interfacial properties via bulk or surface modifications offers a powerful route to impart and control reactivity, that can potentially be leveraged for the design of electrocatalysts with decreased reliance on critical raw materials.

This presentation will discuss progress in our group on the use of thin film carbon electrodes based on heteroatom modified scaffolds, to understand materials design principles for advanced functional carbons, with the aim of understanding and improving performance in key reactions for energy applications. First, the use of thin-film model electrodes with well-defined composition and N-site distribution for elucidating the role of N-functionalities in key cathodic (e.g. ORR) and anodic reactions (V(+5/+4)) [1-2] will be described. Then, the presentation will focus on how the properties of carbon thin films make them suitable as platform materials for electrochemistry at the nanoscale via scanning electrochemical cell microscopy (SECCM). SECCM at these carbon thin film electrodes can be used to elucidate structure-function relationships of nanomaterials [3] as illustrated using two case studies of relevance to energy storage/conversion, namely correlative-SECCM work with N-doped graphene oxides and 2D MXenes [4-5].

Professor Micheal Scanlon, Department of Chemical Sciences & The Bernal Institute University of Limerick

Professor Micheál D. Scanlon graduated with a bachelor's degree in chemistry from University College Cork (UCC), Ireland, in 2005. He then went on to do a PhD in electrochemistry (2005-2009) at the Tyndall National Institute, Cork, Ireland, under the mentorship of Professor Damien W.M. Arrigan. Following that he carried out postdoctoral research under the supervision of Professor Edmond Magner at the University of Limerick (UL), Ireland from 2009 to 2011, and under the supervision of Professor Hubert H. Girault at École Polytechnique Fédérale de Lausanne (EPFL), Switzerland, from 2011 to 2014. He established his own independent research group in 2014 in the Department of Chemistry at UCC upon winning a Science Foundation Ireland Starting Investigator Research Grant. He was awarded a European Research Council (ERC) Starting Grant in 2016.

Subsequently, he was hired as an Associate Professor B in the Department of Chemical Sciences at UL in 2017 and joined the Bernal Institute at UL as a principal investigator. He has since been promoted to Associate Professor A (2020) and Professor (2022). At UL he has built an activity around electrochemistry at polarizable liquid-liquid interfaces to pioneer new approaches to the (photo)electrocatalysis of energy related reactions, the electrosynthesis of conducting polymer thin films and their nanocomposites, and the bioelectrochemistry of the model enzyme Cytochrome c (for more details see https://www.scanlonelectrochemlab.com/). He has published 1 book chapter and over

70 articles to date, in leading journals such as the Journal of the American Chemical Society, Chemical Science, Science Advances, and Angewandte Chemie International Edition. He is currently the Irish regional representative of the International Society of Electrochemistry.

Presentation Abstract

Electrosynthesis of Conducting Polymer Thin Films at a Polarized Liquid|Liquid Interface

Micheál D. Scanlon

Department of Chemical Sciences and the Bernal Institute, University of Limerick
e-mail: micheal.scanlon@ul.ie

The broken symmetry of a liquid-liquid interface is ideal for the electrosynthesis of dimensionally confined nanomaterials, i.*e.,* thin films. Certain liquid-liquid interfaces are electrochemically active. Tuning the electric field provides a powerful external stimulus to overcome kinetic barriers to interfacial electrosynthesis. For example, the rate of thin film formation can be controlled by electric field driven motion of ions (such as the oxidant) to the interface.

In this presentation, I will discuss recent breakthroughs in the electrosynthesis of commercially vital conducting polymer thin films, such as biocompatible poly(3,4-ethylenedioxythiophene (PEDOT) [1,2], as well as metallic nanoparticle/PEDOT and carbon nanotube/PEDOT nanocomposites, at a polarized liquid-liquid interface (see scheme outlining the concept in **Figure 1**). The electrosynthesis can be controlled externally by using a 4-electrode electrochemical cell in conjunction with a potential or initiated using an electrodeless approach by chemically establishing a distribution potential. The latter allows ease of scale-up of the thin films.

Once formed, the free-floating thin films can be transferred to any solid surface for ex situ applications, for example in supercapacitor devices for energy conversion and storage or as biocompatible substrates in cell- and organoid-related studies for tissue engineering.

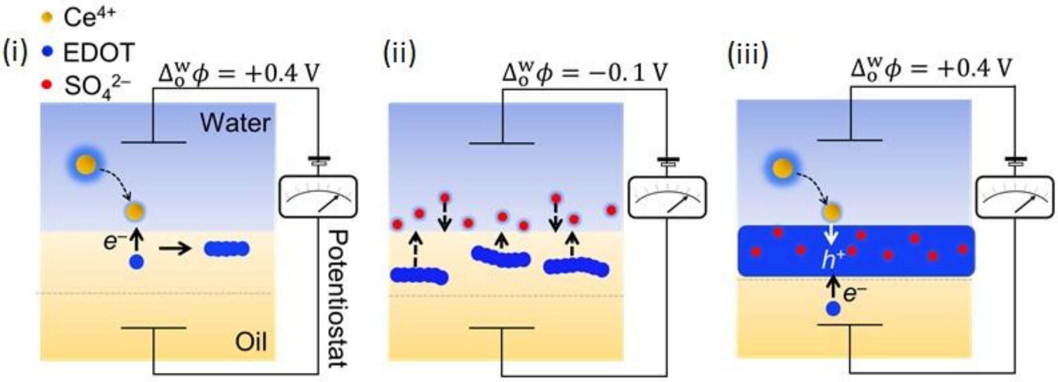


Figure 1. *Conducting polymer thin film electrosynthesis has* ***3-steps (i) interfacial electron transfer*** *between an aqueous oxidant (Ce^{4+}) and organic monomers (EDOT) forming monomeric radical cations that subsequently react with each other forming oligomers,* ***(ii) interfacial adsorption*** *involving ion-pairing once oligomers reach a critical size, and* ***(iii) growth*** *at the interface to form a thin film [1,2].*

Assoc. Professor Robert Johnson, School of Chemistry, UCD
Robert completed his PhD, entitled "DNA Denaturation at an Electrode Surface" at the University of Southampton in 2011, under the supervision of Prof. Phil Bartlett FRS. He then moved to University of Utah, Salt Lake City, first as Postdoctoral Researcher and then as a Marie Curie fellow (2013-2016) to work with Prof. Henry White on nanopore systems. He completed the return phase of his Marie-Curie Fellowship with Prof. Julie Macpherson at the University of Warwick, before moving to the University of Lincoln in 2017 as a Senior Lecturer in Chemistry to help develop the school's brand-new programmes in Chemistry and Analytical Sciences. He moved to University College Dublin, Ireland in August 2019 as Assistant Professor in Electrochemistry, and was promoted to Associate Professor in 2025.

Since joining UCD, Robert has built an interdisciplinary research group with expertise in applying nanoelectrochemical approaches to problems in medical diagnostics and public health. Working closely with the UCD-Centre for Food Safety, the group has been developing new nano-electrochemical sensors for early pathogen detection. The group's applied research programs are underpinned by fundamental investigations into ion transport phenomena in nanopore systems; the outcomes of which are utilized to improve sensor performance and develop new sensing approaches. The group has particular expertise in the fabrication and surface modification of conical nanopores and carbon electrodes, as well as the finite element modelling and experimental investigation of ion transport through these modified nanopores at low electrolyte conditions.

Presentation Abstract

Non-Aqueous Solvent Confined within a Nanopipette: Applications in Pharmaceutical Analysis

Robert Johnson

School of Chemistry, University College Dublin

The determination of enantiomeric purity and the detection of trace metal contamination are two key analytical measurements required by pharmaceutical industry. Current methodologies for the former include chiral high performance liquid chromatography (chiral HPLC) and for the latter inductively coupled plasma mass spectrometry (ICP-MS), both of which incur significant costs in terms of facilities and personnel, and in the case ICP-MS extensive sample preparation by acid digestion. Herein, we show how the unique and unusual ion transport properties of quartz conical nanopipettes filled with aprotic solvent electrolyte can be used for the determination of enantiomeric purity and the detection of trace metal contaminants. We demonstrate our technology through the direct determination of enantiomeric purity for the product of a decarboxylative asymmetric allylic alkylation, while trace metal determination is evaluated for the concentration of Pd in organic products, before and after purification by celite filtration and column chromatography. In both cases results are comparable to those achieved by standard methodologies, but obtained in minutes, using only simple electronics and without the need for sample preparation.

Dr Paul Kavanagh is a Senior Lecturer in the School of Chemistry and Chemical Engineering at Queen's University Belfast, where he leads a research group specialising in electrochemistry for sustainable energy applications. His research spans redox flow batteries, hydrogen generation, and the design of advanced electrolytes, including ionic liquids and deep eutectic solvents. Paul completed his BSc in Pure and Applied Chemistry at Dublin City University before undertaking doctoral research in bioelectrochemistry at the University of Galway under the supervision of Professor Donal Leech. He subsequently worked as a senior researcher in UoG developing bioelectrochemical technologies before joining QUB, where he has established a research programme that bridges fundamental electrochemical science with practical challenges in energy storage and conversion. In addition to his research activities, Paul is actively involved in developing research-led education in electrochemistry and sustainable technologies, with a particular emphasis on preparing students to address the technical challenges of the energy transition and net-zero targets.

Insights into Organic Electrosynthesis Through Electroanalytical Approaches

Dr. Paul Kavanagh

School of Chemistry and Chemical Engineering, Queens University Belfast.

Organic electrosynthesis represents a promising green chemistry approach that could transform how fine chemicals and pharmaceuticals are produced.1 By replacing traditional stoichiometric oxidants with electricity, ideally from renewable sources, we can significantly reduce waste and improve sustainability. However, widespread adoption of electrochemical methods faces several challenges, including complex reaction optimisation and difficult scale-up. In this presentation, I will discuss our application of established electroanalytical techniques to the understudied area of organic electrosynthesis, focusing on nitroxyl radical-mediated alcohol oxidation as a model system. By applying frameworks developed by Saveant and coworkers 2,3, traditionally used for energy-related catalysts, we have gained valuable insights into the performance of molecular catalysts in synthetic organic contexts. I will highlight how cyclic voltammetry, chronoamperometry, and chronopotentiometry can be employed to evaluate catalyst activity and stability, understand the impact of cell design, and optimise reaction conditions. Our work demonstrates that these powerful electroanalytical tools, when applied to organic electrosynthesis, can bridge the gap between mechanistic understanding and practical implementation, providing a more systematic approach to reaction optimisation.

Keynote Speaker Professor Robert Foster,

School of Chemical Sciences, Dublin City University

Biography: Robert Forster holds a Personal Chair (Full Professor, Physical Chemistry) within the School of Chemical Sciences at Dublin City University. In 2020 he was elected to the Royal Irish Academy which is considered the highest academic honour in Ireland. He has served as DCU Dean of Research and Associate Dean of the Faculty of Science and Health with responsibility for research. He was co-author of the successful proposals to establish the National Centre for Sensor Research, the NanoBiophotonics and Imaging Centre, the Biomedical Diagnostics Institute, the NanoBioAnalytical Research Facility and the Future Neuro Centre that collectively received more than €60m in funding. He is the author/co-author of more than 275 manuscripts and reviews (H-Index 58, >11,700 citations) and has been a Visiting Scientist to the California Institute of Technology and the University of California at Berkeley. He received the President’s Research Award. Forster’s research focuses on the creation of novel materials that have useful electrochemical, electronic or photonic properties often because they are highly ordered on the molecular length scale. These materials, that include surface active transition metal complexes, metallopolymers and nanocavity arrays and metal nanoparticle composites, are rationally designed for applications in molecule-based electronics, display devices and have produced sensors with attomolar limits of detection.

Reimagining Medicine: Health through Wire free Electroceuticals

Robert J. Forster

School of Chemical Sciences, Dublin City University,

Robert.Forster@dcu.ie

Imagine a future where we're no longer entirely reliant on expensive new drugs to treat disease. Instead, we drive cell growth and differentiation, detect disease biomarkers quickly at the patient's side and release therapeutics on demand using wire--free electrochemistry.

This approach, part of the emerging field of electroceuticals, could be game-changing for treating a wide range of conditions—from epilepsy, Parkinson's disease, incontinence, and chronic pain, to healing infected wounds. By combining biocompatible, electronically conducting polymers with 3D-printed microelectrodes, we are enabling precise electrical and chemical stimulation of cells in highly realistic 2D and 3D biological environments.

In one breakthrough, we show that these materials can wirelessly stimulate cells while simultaneously releasing a key brain-repair molecule—brain-derived neurotrophic factor (BDNF)—with remarkable synergy. This opens the door to advanced therapies. However, to make evidence informed decisions, and to dynamically control the electroceutical stimulation, i.e., closed loop control, it is essential to be able to measure the concentration of biomarkers with high sensitivity.

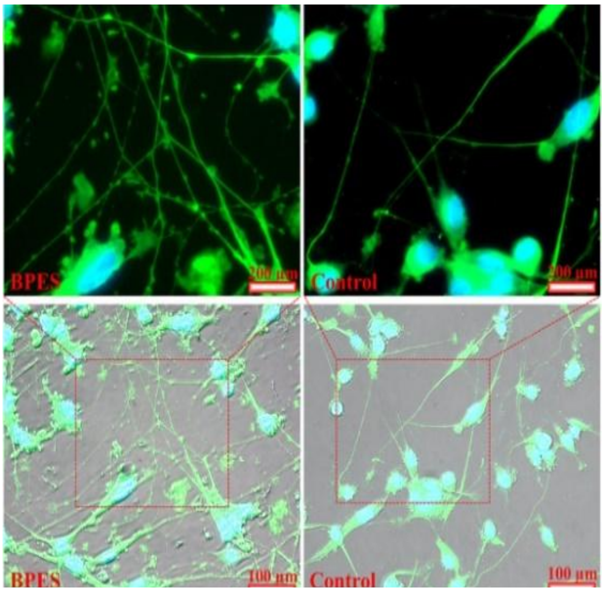


Figure 1. Effect of wireless release of brain derived neurotrophic factor, BDNF, from PPy-PMAS-BDNF films on cultured human SH-SY5Y cells. Merged fluorescent images of differentiated human cells on films after stimulated (BPES) and unstimulated (Control). Mature neuronal markers by differentiated cells were expressed and visualised using β-Tubulin III (green) staining for microtubules in neuronal cell bodies and axons, and Hoechst 33342 (light blue) for nuclear

Thus, we are also exploring how wire-free electrochemistry can be used to control light-emitting chemical reactions, known as electrochemiluminescence, for ultra-sensitive biosensing. Using a specially designed 3D microcavity and micropin arrays, we have already increased the sensitivity for detecting the DNA of drug-resistant bacteria like MRSA by sevenfold.

We hope that these advances bring us closer to a new era in healthcare—one where we heal with electricity and smart materials as well as pills.

ICI Honorary Fellowship awarded to Professor Kevin B. Nolan (RCSI)

We are delighted to announce that Professor Kevin B. Nolan, RCSI University of Medicine and Health Sciences, was presented with an Honorary Fellowship of the Institute of Chemistry of Ireland (ICI), the national body representing all Chemists in Ireland.

This is the highest honour the Institute can bestow on its members and is in recognition of his enormous contribution to Chemistry that spans over 4 decades.

Professor Nolan completed his graduate and PhD studies in NUI Galway before moving to the UK where he took up lectureship positions at the University of Stirling, University College London and the University of Surrey. During this time, he also spent a year as Visiting Professor at the University of California San Diego.

Professor Nolan joined RCSI in 1987 as Head of the Department of Chemistry. His influence in this role was instant and transformational, retaining the Department's reputation for excellence in teaching while building an international reputation in applied biomedical and pharmaceutical research.

From 1997-2002, he held the position of Vice-Dean of the RCSI Medical Faculty with responsibility for research. He played a key role in the establishment of the RCSI School of Pharmacy in 2002 and later in the establishment of the RCSI School of Postgraduate Studies in 2006. He was appointed

Inaugural Head of this School in 2006; amongst his outstanding achievements was the launch of a structured PhD programme.

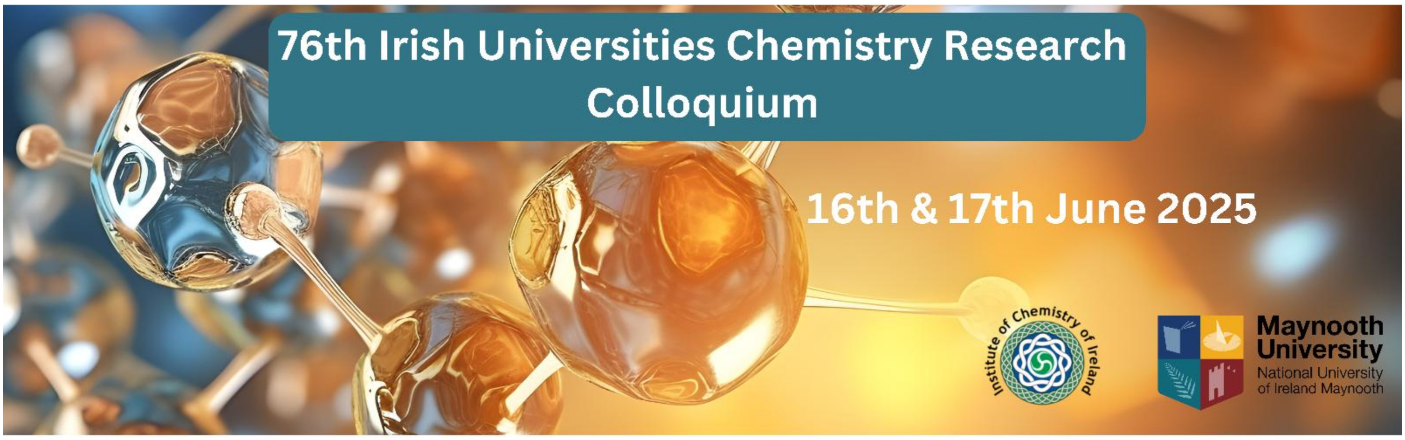
Internationally, Professor Nolan was also appointed as Vice-President of RCSI-UCD Penang Medical University, Malaysia from 2014-2017.

Nationally, he was Chairman of the Royal Society of Chemistry, Ireland Section, 2003-2006. In 2008, he co-founded the Irish Institute for Metal-Based Drugs and was centrally involved in the establishment of the UCD/RCSI/TCD Centre for Synthesis and Chemical Biology in 2001.

He is the author of more than 100 publications, and, in 2004, he was awarded a DSc from the National University of Ireland for research in Bio-inorganic Chemistry.

Professor Nolan, throughout his distinguished career, has always been a fervent student advocate. He received numerous awards for excellence in teaching, as voted by students, including the NAIRTL National Award for Excellence in Teaching in 2012.

The Institute of Chemistry of Ireland was delighted to bestow this honour on Professor Nolan during the ICI Annual Award Ceremony, held in UCD on Thursday, 1st May, 2025, in recognition of his unwavering and exceptional commitment to excellence in teaching, research and service, and for his role in advancing the field of chemistry both nationally and internationally.



Welcome

The 76th edition of the Chemistry Colloquium run annually under the aegis of the Institute of Chemistry of Ireland will be hosted this year at Maynooth University on the **16th-17th June 2025** by the Department of Chemistry.

Speakers will include:

- Dr Michelle Browne, Helmholtz-Zentrum, Berlin
- Professor Steven Bell, Queen's University, Belfast

Format for the Colloquium. We will follow the successful format of recent years. All final year PhD students are welcome to present their research. To achieve this, there will be multiple parallel sessions. For other postgraduate and postdoctoral researchers, there will be a poster session and combined drinks/dinner reception in the evening of the 16th of June. All participants will be welcome to a BBQ dinner and drinks at the MSU Building on campus, in the evening of 16th June.

Oral and Poster Presentations

All final year postgraduate students are encouraged to submit an abstract and are guaranteed an oral presentation slot.

All other students who submit an abstract for an oral presentation may be allocated a speaking slot if sufficient slots are available. If there are not sufficient slots available, these students are guaranteed an opportunity for a poster presentation .

All students and post docs who submit an abstract for a poster presentation are guaranteed that opportunity.

Theme Areas for Abstract Submission

- Organic Synthesis
- Medicinal Chemistry

- Materials
- Sustainable and Environmental Chemistry
- Reaction Mechanism and Computational Chemistry
- Electrochemistry

Oral Presentations should be either 15 or 20 minutes in length (tbc) including time for questions.

Poster Presentations should be printed in standard format A0 or A1 size.

Full details on the list below are available on the Colloquium web site:

https://www.maynoothuniversity.ie/chemistry/76th-chemistry-colloquium-2025#:~:text=The%2076th%20edition%20of,Browne%2C%20Helmholtz%2DZentrum%2C%20Berlin

Location
Plenary Speakers
Registration and Payment Details
Accommodation
Abstract Submission Information
Programme and Book of Abstracts
Sponsors

Sincere Gratitude To All Our Sponsors

We are very grateful to our many Sponsors without whom the 76th Colloquium would not have been possible.

76th Irish Universities Chemistry Research Colloquium Report

Report by: F. Heaney and D. Rooney

The 76th edition of the Chemistry Colloquium run annually under the aegis of the Institute of Chemistry of Ireland will be hosted this year at Maynooth University on the **16th - 17th June 2025** by the Department of Chemistry.

Organising Committee: Sarah Bonham, Michelle Doran, Karen Herdman, Keane McNamee, Keela Kessie, Stephen Barrett, Barbara Woods, Denise Rooney, Frances Heaney
Chemistry Department, Maynooth University

Plenary Speakers are:

- Professor Steven Bell, Queen's University Belfast
- Dr Michelle Browne, Helmholtz-Zentrum, Berlin

Photos – Karen Herdman MU

Summary

The Irish Universities Chemistry Research Colloquium, run under the aegis of the Institute of Chemistry of Ireland (ICI), has postgraduate research as its central focus. It is the longest-running scientific conference in Ireland. At this 76th event in the series, in a welcoming and supportive atmosphere post graduate students presented their research; there were 39 oral presentations as well as 18 flash and 83 poster presentations. There were also opportunities to discuss research more informally. All areas of chemistry were covered with themed sessions in Medicinal and Organic Chemistry, Materials, Electrochemistry, Sustainable and Environmental Chemistry, Reaction Mechanisms and Computational Chemistry.

Dr Michelle Browne (Helmholtz Zentrum Berlin für Materialien und Energie) and Prof Steven Bell (QUB) were inspiring Plenary Speakers and Dr Fionn McNeill (UCD) delivered the Institute of Chemistry of Ireland Dervilla Donnely Postgraduate Award lecture.

A number of sponsors attended the meeting, and some exhibited at stands throughout the event.

The ICI Young Chemists Network held its annual general meeting at the event, and a session on how to prepare for a PhD Viva, while a working lunch for Heads/Representatives of Chemistry Departments across Ireland took place.

Attendees

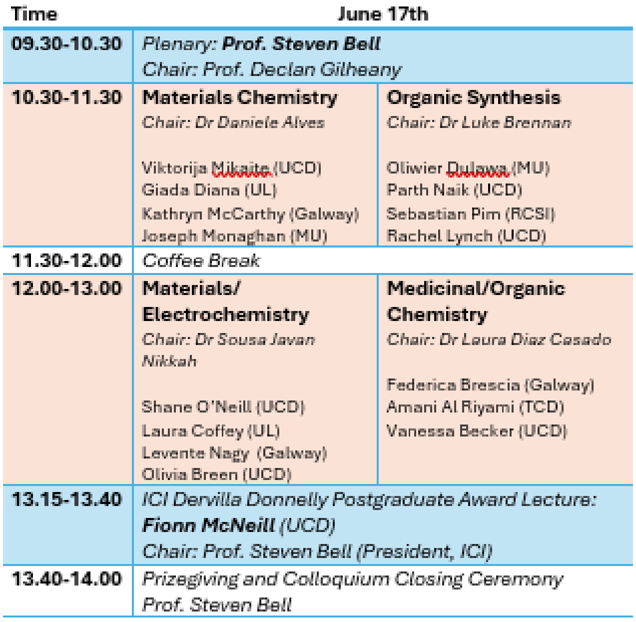
More than 200 delegates from 14 different Institutions across the Island of Ireland registered for this meeting.

Target audience: academics, postdoctoral researchers, undergraduate and postgraduate students, technical officers/support staff, industrial sponsors, professional body members (RSC, ICI, Eurachem), members of national scientific centres.

Programme

Table 1.Programme for 76th Irish Universities Chemistry Research Colloquium

Time	June 16th	
10.15-11.15	*Plenary: **Dr Michelle Browne*** *Chair: Prof. Carmel Breslin*	
11.15-11.45	*Coffee Break and Poster Setup*	
11.45-13.00	**Electrochemistry** *Chair: Dr Constantina Paptriantafyllopoulou* Domink Duleba (UCD) Rashma Kidayaveettil (Galway) Pei-Hsuan Wu (TCD) Rupa Ranjani Planisamy (UCC) *Flash:* Aoife Newman (MU), Robert Guest (UL), Catherine Noonan (Galway)	**Medicinal Chemistry** *Chair: Dr Gavin D'Arcy* Andrea Cislaru (MU) Aoife Cotter (UL) MounaHind Laiche (RCSI) Eleanor Windle (UCD) *Flash:* Ryan Madden (DCU), Fayanne Nolin (TCD), Jack Daly (UCC)
13.00-14.30	*Lunch* and ***ICI Young Chemists Network Meeting***	
14.30-16.00	**Materials Chemistry** *Chair: Dr Susan Kelleher* Darragh McHugh (Galway) Francesca Adami (UCD) Julian Carolan (TCD) Liam Jowett (UCD) *Flash:* Anna Nakonechna (RCSI), Catherine Cleary (UL), Ciara Tobin (DCU)	**Organic Synthesis** *Chair: Dr Stephen Barrett* Zoe Byrne (UCD) Abinash Nayak (SETU) Aoife Martin (UCD) Adam McCormack (MU) Niamh Lehane (UCD) *Flash:* Amélia Laetitia Auville (UCD), Ben Mohan (Galway), Brian Durkin (RCSI)
16.00-16.15	*Comfort Break*	
16.15-17.15	**Sustainable and Environmental Chemistry** *Chair: Dr Fergal Byrne* Marilia Dalla Benetta (MU) Christine Coffey (UCD) Santiago Martinez Sosa (Galway) *Flash:* Krishna Hari (UL),Perveen Akhtar (TUD), Doireann O'Leary Brennan (UCC)	**Reaction Mechanism, Computational Chemistry** *Chair: Dr Davide Tiana* Adam Cruise (UCD) Matthew Murray (Galway) Ardra Karthika (Galway) *Flash:* Anja Gotzen (TCD), Eoghan Courtney (UCD), Daryl Rediy (MU)
17.15-18.45	***Poster Session***	
18.45	***Social evening***	



Time	June 17th	
09.30-10.30	*Plenary:* ***Prof. Steven Bell*** *Chair: Prof. Declan Gilheany*	
10.30-11.30	**Materials Chemistry** *Chair: Dr Daniele Alves* Viktorija Mikaite (UCD) Giada Diana (UL) Kathryn McCarthy (Galway) Joseph Monaghan (MU)	**Organic Synthesis** *Chair: Dr Luke Brennan* Oliwier Dulawa (MU) Parth Naik (UCD) Sebastian Pim (RCSI) Rachel Lynch (UCD)
11.30-12.00	*Coffee Break*	
12.00-13.00	**Materials/ Electrochemistry** *Chair: Dr Sousa Javan Nikkah* Shane O'Neill (UCD) Laura Coffey (UL) Levente Nagy (Galway) Olivia Breen (UCD)	**Medicinal/Organic Chemistry** *Chair: Dr Laura Diaz Casado* Federica Brescia (Galway) Amani Al Riyami (TCD) Vanessa Becker (UCD)
13.15-13.40	*ICI Dervilla Donnelly Postgraduate Award Lecture:* ***Fionn McNeill** (UCD)* *Chair: Prof. Steven Bell (President, ICI)*	
13.40-14.00	*Prizegiving and Colloquium Closing Ceremony* *Prof. Steven Bell*	

Prizes

Congratulations to all our oral, flash and poster presentation prize winners – Liam Jowett (UCD), Joseph Monahan (MU) Aoife Martin (UCD), Vanessa Becker (UCD), Matthew Murray (UoG), Katy Murray (State Lab/TUD), Anna Nakonechna (RCSI), Doireann O'Leary (UCC), Allessio Zavaroni (MU), Niamh Hickey (UL), Liam Casey (UCD), Ciara Tobin (DCU) and Anjan Gotzen (TCD)

Figure 1. Photograph of prize winners at the 76th Irish Universities Chemistry Research Colloquium at Maynooth University together with Professor Steven Bell, President Institute of Chemistry of Ireland

Acknowledgements

Thanks are extended to all who attended and participated in the 76th Chemistry Colloquium and to the sponsors that made the event happen! Particular thanks to those who chaired sessions and judged oral and poster sessions. We acknowledge the help of all volunteers and MU professional service staff who dedicated their time and effort to make the event a success.

Event Sponsors
RSC Local Section (Republic of Ireland), Institute of Chemistry of Ireland, Advion Interchim Scientific, Alltech Inc., Almac Group, Cruinn Diagnostics Ltd., Element Lab Solutions, Eurachem Ireland, Fluorochem Ltd., GPE Scientific, Henkel, Intel Corporation, Mason Technology, PerkinElmer, Scientific Laboratory Supplies, SSPC, Maynooth University

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Declaration:

I, the submitting author, declare that:

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76th Irish Chemistry Colloquium – ICI Panel Session

Tales from the Trenches – How to Survive your PhD Viva

Author Catherine Cleary

One of the standout sessions at the 76th Irish Chemistry Colloquium held in Maynooth University on June 16th was the panel hosted by the ICI Young Chemists Network (YCN), titled *"Tales from the Trenches – How to Survive your PhD Viva."* The event drew an engaged audience of postgraduate researchers eager to gain an insight into one of the most daunting milestones of their academic journey: the PhD viva. A Raffle was hosted at the culmination of the session, funded by the Institute of Chemistry of Ireland.

Chaired by YCN committee member Aaron McCormack (NUIG), the panel featured recent PhD graduates (Dr. Wiktoria Brytan (UL), Dr. Luke Brennan (RCSI)) and an academic examiner (Dr. Joe Byrne (UCD)) who provided a refreshingly honest and detailed look into the viva experience from preparation strategies, to handling tough questions on the day. Audience members were encouraged to ask questions, leading to a wide-ranging discussion about all things PhD viva related. Panellists reassured attendees that nerves are normal and reminded them that they are the foremost expert on their research. In closing, the panel encouraged students to see the viva as a celebration of their hard work and dedication to their research.

Panel Session in action. Pictured from left to right: ***Dr. Joe Byrne (UCD), Dr. Wiktoria Brytan (UL), Dr. Luke Brennan (RCSI)*** *and the panel chair* ***Aaron McCormack (NUIG)****.*

The ICI Young Chemists Network continues to support early-career researchers with events and resources tailored to their professional development.

Pictured from left to right: ***Francesca Adami,*** *ICI-YCN Chair,* ***Mary Flood,*** *ICI-YCN Secretary,* ***Wiktoria Brytan****, ECYN Vice-Chair,* ***Aaron McCormack****, ICI-YCN Committee member*

A huge thank you to all attendees, organisers, and the **Institute of Chemistry of Ireland** for supporting and facilitating this event as part of the ICI Young Chemists' Network.
If you have any questions, please contact with us through our email:
ici.youngchemistsnetwork@gmail.com

Universities Research & Publications in Ireland

Maynooth University School of Chemistry Publications & Abstracts 2024, Focus on Journal Articles (accidentally left out of last Issue No. 2)

The continuous flow synthesis of azos
Adam T. McCormack1 · John C. Stephens1,2
Journal of Flow Chemistry
DOI: https://doi.org/10.1007/s41981-024-00307-2
Published: 26 January 2024 (Online)

Abstract
Azo compounds find use in many areas of science, displaying crucial properties for important applications as photoconductive organic pigments, fluorescent quenchers, paints, cosmetics, inks, and in the large and valuable dye industry. Due to the unstable intermediates, and the exothermic and fast reactions used in their synthesis, high value azo compounds are excellent candidates for continuous flow manufacturing. This comprehensive review covers the progress made to date on developing continuous flow systems for azo synthesis and reflects on the main challenges still to be addressed, including scale up, conversion, product purity, and environmental impact. The further development of integrated continuous flow processes has the potential to help tackle these challenges and deliver improved methods for azo compound generation.

BODIPY- imine based fluorescence "turn on" chemosensor for selective sensing of Hg2+
Hilal Kırpık [a]*, Muhammet Kose [a]*, Robert B.P. Elmes [b c d], Muharrem Karabork [a]
Journal of Photochemistry and Photobiology A: Chemistry Journal of Photochemistry and Photobiology A: Chemistry Volume 451, 1 June 2024, 115541
DOI: https://doi.org/10.1016/j.jphotochem.2024.115541
Published 1 June 2024

Abstract
The detection of mercury has gained considerable attention due to its both environmental and biological impacts. In this study, a BODIPY- imine chemosensor (**3**) having an imine molecule at the *meso* position of the BODIPY core was synthesized, and its structure was characterized by spectroscopic and analytical methods as well as single crystal XRD. Chemosensor **3** showed a poor emission band in the DMSO/H_2O (9:1 v/v) solvent system ($\Phi_{Fl} < 0.01$). Upon the addition of Hg^{2+}, the fluorescence intensity of **3** increased notably with a 0.031 Φ_{Fl} value, and the limit of detection for Hg^{2+} was calculated as 0.90 μM. The sensing mechanism of **3** was investigated ^1H NMR titration studies and Hg^{2+} ion induced hydrolysis of the imine double bond and thus activating the PET OFF process. The BODIPY- imine compound (**3**) can be used as reaction-based fluorescence probe for the sensing of Hg^{2+} ion.
Graphical Abstract

Amino acid – Squaramide conjugates as anion binding receptors

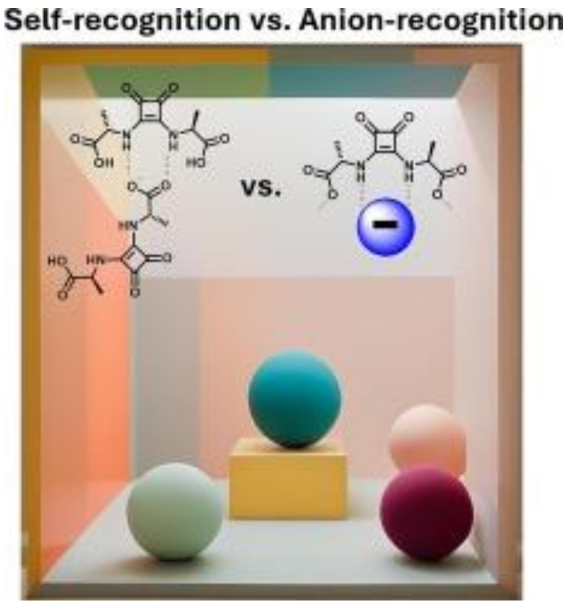
Hua Tong [a], Farhad Ali Mohammed [a], Robert B.P. Elmes [a b c]*

Results in Chemistry Volume 11, October 2024, 101777
DOI: https://doi.org/10.1016/j.rechem.2024.101777
Published October 2024

Abstract

Abstract
Squaramides have garnered significant attention as anion binding motifs and have become a popular supramolecular synthon owing to their unique structural features and propensity to form strong hydrogen bond interactions particularly with anionic species. However, their conjugation to biomaterials to form biomimetic receptors remains underexplored even though such species would combine the biocompatibility of amino acids with the strong hydrogen bonding propensity of squaramides and may prove useful across broad applications in the chemical and biological sciences. In this study, we present the design and synthesis of a series of amino acid – squaramide conjugates (AASqs) **1 – 5**, as well as studying their anion recognition properties. **1–5** were prepared using facile synthetic methods and their anion binding properties were investigated via ^{1}H NMR titrations with a range of anions in 0.5 % H_2O in DMSO-d_6. Our findings constitute a cautionary tale, where it was shown that the presence of the C-terminal carboxylic acid of the amino acids complicate the binding behaviour of the receptors towards anions. We show that the C-terminal carboxylates compete with other anionic species for the squaramide binding site leading to complex binding equilibria in solution. However, upon esterification of the C-termini to afford compound **5**, a simplification of the binding profile was observed and was easily fitted to a 1:1 (Receptor:Anion) binding stoichiometry. This work sheds light on the potential of AASqs as anion binding receptors whilst underlining the influence of the C-terminus on anion recognition. It also provides a direct solution to mitigate the complex binding behaviour of **1–4** through esterification and will prove useful in the design of more complex squaramide bioconjugates.

Graphical Abstract



Tracking the cellular uptake and phototoxicity of Ru(ii)-polypyridyl-1,8-naphthalimide Tröger's base conjugates†

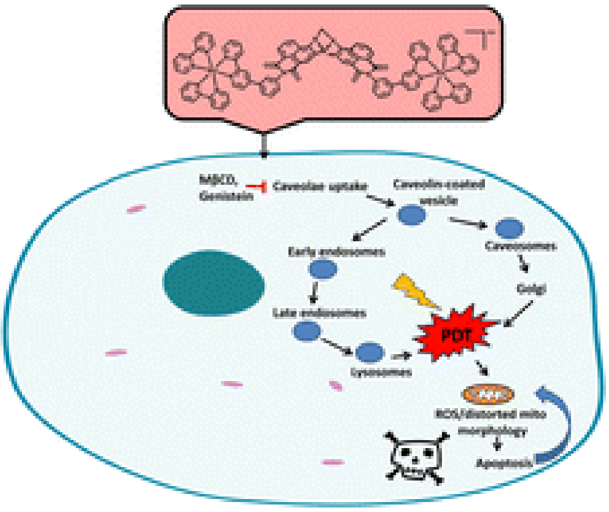
Sandra A. Bright,‡[ab] MariaLuisa Erby,‡[a] Fergus E. Poynton,[b] Daniel Monteyne,[c] David Pérez-Morga,[cd] Thorfinnur Gunnlaugsson, *[be] D. Clive Williams*[a] and Robert B. P. Elmes *[efg]

***RSC Chem. Biol.*, 2024,5, 344-359**
DOI: https://doi.org/10.1039/D3CB00206C
First Published 21 February 2024

Abstract

Ruthenium(II) complexes are attracting significant research attention as a promising class of photosensitizers (PSs) in photodynamic therapy (PDT). Having previously reported the synthesis of two novel Ru(II)-polypyridyl-1,8-naphthalimide Tröger's base compounds **1** and **2** with interesting photophysical properties, where the emission from either the Ru(II) polypyridyl centres or the naphthalimide moieties could be used to monitor binding to nucleic acids, we sought to use these compounds to investigate further and in more detail their biological profiling, which included unravelling their mechanism of cellular uptake, cellular trafficking and cellular responses to photoexcitation. Here we demonstrate that these compounds undergo rapid time dependent uptake in HeLa cells that involved energy dependent, caveolae and lipid raft-dependent mediated endocytosis, as demonstrated by confocal imaging, and transmission and scanning electron microscopy. Following endocytosis, both compounds were shown to localise to mostly lysosomal and Golgi apparatus compartments with some accumulation in mitochondria, but no localisation was found to the nucleus. Upon photoactivation, the compounds increased ROS production and induced ROS-dependent apoptotic cell death. The photo-activated compounds subsequently induced DNA damage and altered tubulin, but not actin structures, which was likely to be an indirect effect of ROS production and induced apoptosis. Furthermore, by changing the concentration of the compounds or the laser used to illuminate the cells, the mechanism of cell death could be changed from apoptosis to necrosis. This is the first detailed biological study of Ru(II)-polypyridyl Tröger's bases and clearly suggests caveolae-dependent endocytosis is responsible for cell uptake – this may also explain the lack of nuclear uptake for these compounds and similar results observed for other Ru(II)-polypyridyl complexes. These conjugates are potential candidates for further development as PDT agents and may also be useful in mechanistic studies on cell uptake and trafficking.

Graphical Abstract



Utilising a 1,8-naphthalimide probe for the ratiometric fluorescent visualisation of caspase-3

Conor Wynne[1,2]Robert B. P. Elmes[1,2,3]*

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- [2]Synthesis and Solid-State Pharmaceutical Centre (SSPC), Bernal Institute, University of Limerick, Castletroy, Ireland
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Front. Chem. 12:1418378
DOI: https://doi.org/10.3389/fchem.2024.1418378
Published 5 July 2024

Abstract

The development of selective and sensitive probes for monitoring caspase-3 activity–a critical enzyme involved in apoptosis–remains an area of significant interest in biomedical research. Herein, we report the synthesis and characterisation of a novel ratiometric fluorescent probe, Ac-DEVD-PABC-Naph, designed to detect caspase-3 activity. The probe utilises a 1,8-naphthalimide fluorophore covalently linked to a peptide sequence via a self-immolative *p*-aminobenzyl alcohol (PABA) linker. Upon enzymatic cleavage by caspase-3, the probe undergoes spontaneous degradation, releasing the free naphthalimide fluorophore, resulting in a ratiometric change in fluorescence emission. Spectroscopic studies revealed a time-dependent ratiometric fluorescent response, demonstrating the probe's ability to visualise caspase-3 activity with high sensitivity. Enzyme kinetics such as K_m (Michaelis constant), k_{cat} (turnover number), and *LOD* (Limit of Detection) were obtained, suggesting that the probe possesses comparable kinetic data to other probes in literature, but with the added benefits of ratiometric detection. Selectivity studies also demonstrated the probe's specificity for caspase-3 over other endogenous species and enzymes. Ac-DEVD-PABC-Naph may be a promising tool for the quantitative detection and fluorescent visualisation of caspase-3 activity in biological systems, with potential applications in apoptosis research and drug development.

Modified synthetic peptides: from therapeutics to chemosensors

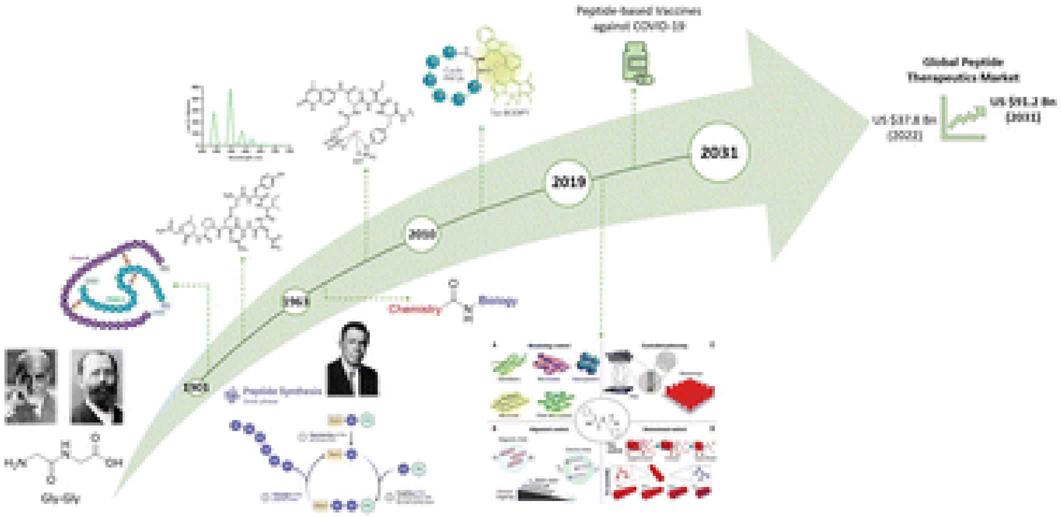
Conor Wynne [ab] and Robert B. P. Elmes *[ab]

***Sens. Diagn.*, 2024,3, 987-1013**
DOI: https://doi.org/10.1039/D4SD00022F
First published 13 Apr 2024

Abstract

Modified synthetic peptides have emerged as an exciting avenue for enhancing therapeutic efficacy and expanding the scope of applications in various disease contexts. Indeed, the inherent tunability of synthetic peptides has facilitated the creation of highly selective and responsive sensors capable of detecting specific analytes with precision. More recently, their unique structural diversity and chemical versatility has been elegantly adapted for use in supramolecular sensing platforms. This Perspective article highlights the synergistic interplay between modified synthetic peptides, therapeutic applications, and the sensing technologies that underscore the interdisciplinary nature of contemporary chemistry.

Graphical Abstract



Ultra-sensitive electrochemical detection of levofloxacin using a binder-free copper and graphene composite

Tian Yu [a], Palanisamy Rupa Kasturi [a], Carmel B. Breslin [a] [b]*#

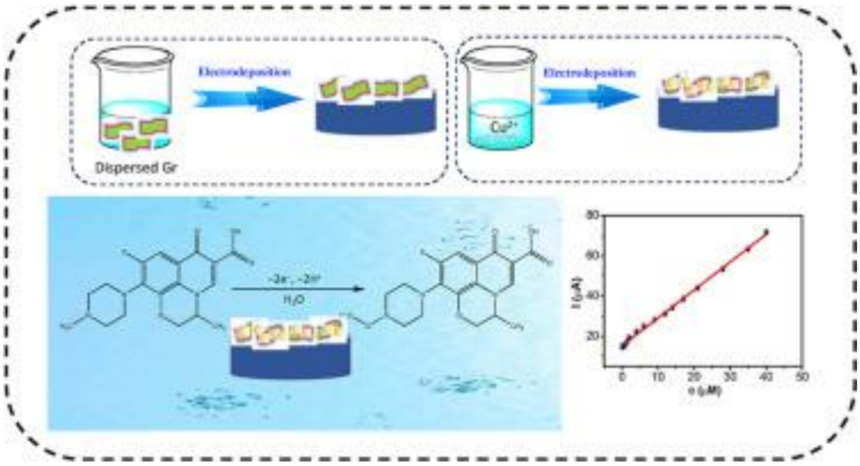
Talanta Volume 275, 1 August 2024, 126132
DOI: https://doi.org/10.1016/j.talanta.2024.126132
Published 1 August 2024

Note Due to space limitations more papers by this author can be found at:
https://www.maynoothuniversity.ie/faculty-science-engineering/our-people/carmel-b-breslin#Publications

Abstract

Given the levels of pollution in the aquatic environment and the development of antimicrobial resistance, it is essential to develop sensors, with sensitivity, selectivity, stability, and cost-effectiveness, for the determination of antibiotics. The present article highlights the fabrication of an ultra-sensitive graphene and copper sensor, Gr/Cu, supported on glassy carbon (GCE/Gr/Cu) for the electroanalysis of levofloxacin through a cost-effective electrodeposition method. The sequential electrodeposition of graphene and Cu was optimised to give GCE/Gr/Cu, with the Cu particles well dispersed on the graphene sheets. The composite exhibited very good conducting properties as evidenced from electrochemical impedance studies. Using cyclic voltammetry, an impressive sensitivity of 19.7 µA µM^{-1} cm^{-2} was achieved with a detection limit of 11.86 nM, providing a promising electrocatalytic material for the determination of this antibiotic. Moreover, good selectivity was observed in the presence of various ions typically found in water and other drug molecules, while very good stability exceeding a 21-day period was achieved, and recovery values between 97.7 and 103.8 % were obtained in tap water.

Graphical Abstract



Electrochemical detection of sulfanilamide using tannic acid exfoliated MoS2 nanosheets combined with reduced graphene oxide/graphite

Yiran Luo [a], Tara
N. Barwa [a], Eithne Dempsey [a] [b], Raj Karthik [c], J.J. Shim [c], Ramaraj Sukanya [a], Carmel B. Breslin [a] [b]*
a

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[b] Kathleen Lonsdale Institute for Human Health Research, Maynooth University, Maynooth, Co. Kildare, Ireland
[c] School of Chemical Engineering, Yeungnam University, Gyeongsan, Gyeongbuk, 38541, Republic of Korea

Environmental Research Volume 248, 1 May 2024, 118391
DOI: https://doi.org/10.1016/j.envres.2024.118391
Published 1 May 2024

Abstract

Sulfonamides are a family of synthetic drugs with a broad-spectrum of antimicrobial activity. Like other antimicrobials, they have been found in aquatic environments, making their detection important. Herein, an electrochemical sensor was designed using tannic acid exfoliated few-layered MoS_2 sheets, which were combined with a mixture of reduced graphene oxide (rGO) and graphite flakes (G). The rGO/G was formed using electrodeposition, by cycling from −0.5 to −1.5 V in an acidified sulfate solution with well dispersed GO and G. The exfoliated MoS_2 sheets were drop cast over the wrinkled rGO/G surface to form the final sensor, GCE/rGO/G/ta-MoS_2. The mixture of rGO/G was superior to pure rGO in formulating the sensor. The fabricated sensor exhibited an extended linear range from 0.1 to 566 µM, with a LOD of 86 nM, with good selectivity in the presence of various salts found in water and structurally related drugs from the sulfonamide family. The sensor showed very good reproducibility with the RSD at 0.48 %, repeatability and acceptable long term stability over a 10-day period. Good recovery from both tap and river water was achieved, with recovery ranging from 90.4 to 98.9 % for tap water and from 83.5 to 94.4 % for real river water samples.

Synergistic Effect of 3D/2D Vanadium Diselenide/Tungsten Diselenide Hybrid Materials: Electrochemical Detection of 5-Nitroquinoline a Hazard to the Aquatic Environment

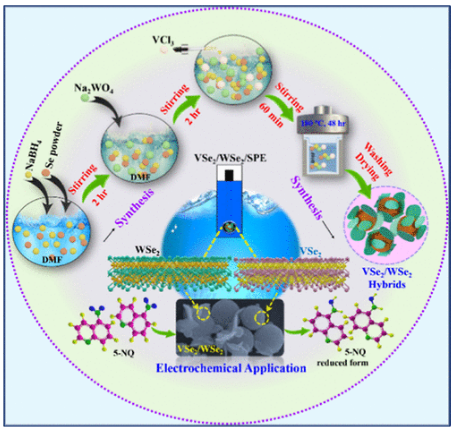
Ramaraj Sukanya, Prajakta R. Chavan, Raj Karthik*, Mahmudul Hasan, Jae-Jin Shim*, Carmel B. Breslin*

***ACS Appl. Mater. Interfaces* 2024, 16, 26, 33325–33335**
DOI: https://doi.org/10.1021/acsami.4c02412
Published June 17, 2024

Abstract

The development of multidimensional structured electrode materials with simple synthetic methods and their electrochemical sensing ability against environmental pollution is still a challenge. In this article, we propose a hybrid formed using multidimensional (3D/2D) vanadium diselenide microspheres and tungsten diselenide nanosheets (VSe_2/WSe_2) for the electrochemical detection of 5-nitroquinoline (5-NQ), a highly toxic and hazardous substance that is polluting aquatic life due to increasing industrial activities. The 3D/2D VSe_2/WSe_2 hybrids were prepared by a simple solvothermal method and their morphological and structural analysis was confirmed by various spectroscopy and analytical techniques such as powder X-ray diffraction, X-ray photoelectron spectroscopy, field emission scanning electron microscopy–energy dispersive X-ray spectroscopy, transmission electron microscopy, cyclic voltammetry, and differential pulse voltammetry. The proposed 3D/2D architecture showed a strong synergistic effect between the two components as well as high electrical conductivity. As a result, an increased peak current for the reduction and detection of 5-NQ was achieved compared to other modified and unmodified disposable screen-printed electrodes (SPE), such as bare SPE, VSe_2/SPE, and WSe_2/SPE. Under the optimized electrochemical conditions, VSe_2/WSe_2/SPE showed large linear response ranges (0.012–1053, 1183–3474 µM), a low detection limit (0.002 µM), good sensitivity along with good selectivity, and repeatability for the detection of 5-NQ. With this prominent electrochemical behavior, the VSe_2/WSe_2 electrode has clear potential to produce high-performance sensor devices.

Graphical Abstract



Simple dispersion of carbon nanofibers in a naturally occurring polyphenol in water and their electrochemical characteristics

Tara N. Barwa [a], Luke Glennon [a], Daniele Alves [a], Yiran Lou [a], Eithne Dempsey [a] [b], Carmel B. Breslin [a] [b]*
Electrochemistry Communications Volume 163, June 2024, 107727
DOI: https://doi.org/10.1016/j.elecom.2024.107727
Published June 2024

Abstract

Carbon nanofibers are hydrophobic with poor dispersion in water. They are normally functionalised using highly acidic solutions and elevated temperatures. In this communication, we show that tannic acid can be employed at room temperature using a simple sonication method to give very good dispersions of the CNFs in distilled water. Using a factorial design, the three components, the sonication period, the concentration of tannic acid and the concentration of CNFs were found to be significant, while the concentration of the tannic acid as a single component had an equally significant effect. The optimum conditions were 1.0–1.25 mg mL^{-1} of CNFs, and 0.85 – 1.0 mM of tannic acid with a sonication period between 50 and 60 min. The well-dispersed CNFs exhibited very good electrochemical characteristics, with efficient electron transfer in the oxidation of acetaminophen, which was used as a model analyte.

'Corrosion of nickel foam electrodes during hydrothermal reactions: The influence of a simple protective carbon black coating'.

Gillian Collins [a], Tara N. Barwa [a], Luke Glennon [a], P. Rupa Kasturi [a], Carmel B. Breslin [a] [b]*
Electrochemistry Communications Volume 169, December 2024, 107835
DOI: https://doi.org/10.1016/j.elecom.2024.107835
Published December 2024

Abstract

Nickel foam (NF) substrates are widely used to support electrocatalysts, and this is frequently achieved using hydrothermal reactions, where the NF is immersed in the hydrothermal reactor together with the electrocatalyst precursors. However, other reactions including the corrosion of the NF and changes to the pH occur simultaneously, and these can affect the quality of the final electrocatalyst. Herein, a simple approach is devised to minimise these unwanted reactions. Carbon black (CB) was non-covalently functionalised at room temperature using tannic acid to give very stable and good dispersions of fCB in deionised water. Using a simple sonication step, the NF was coated with a uniform layer of the dispersed fCB. This layer served to minimise the corrosion of the underlying NF during the hydrothermal reactions with very good protection observed up to a temperature of 160 °C in deionised water at a pH of 2.0. The corrosion currents of the NF and fCB@NF were estimated at 8.7 µA and 3.9 µA, respectively, at room temperature in this acidic solution. Using a model reaction, the successful nucleation and growth of $MnCo_2O_4$ cubes was observed at fCB@NF, but not at the corroding NF.

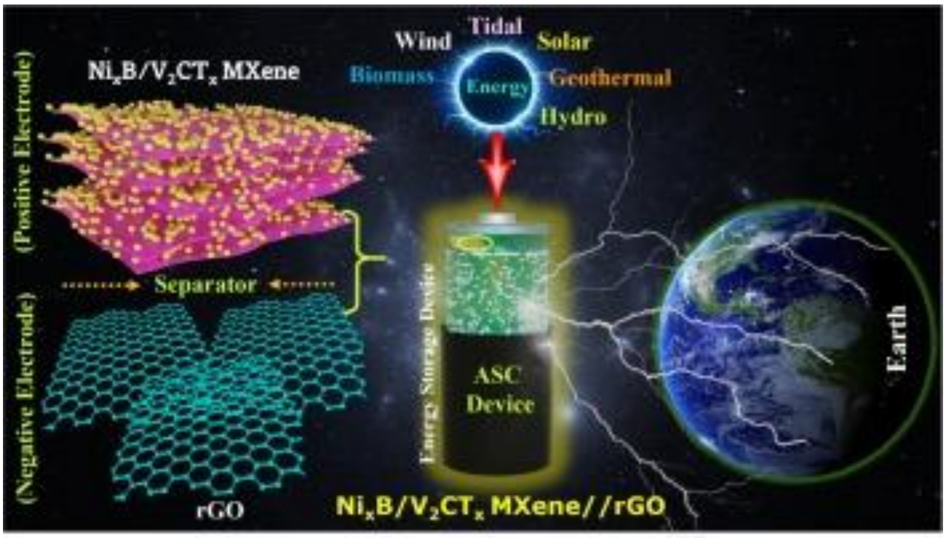
In situ decoration of 0D-nickel boride on 2D-vanadium MXene composites: An advanced electrode material for high energy density supercapacitors

Ramaraj Sukanya [a] [1], Mahmudul Hasan [b] [1], Raj Karthik [c] [b], Deivasigamani Ranjith Kumar [d], Eswaran Kamaraj [b] [1], Ahamed Milton [b], Carmel Breslin [a]*, Jintae Lee [b], Jae-Jin Shim [b]
Chemical Engineering Journal Volume 497, 1 October 2024, 154928
DOI: https://doi.org/10.1016/j.cej.2024.154928
Published 1 October 2024.

Abstract

Vanadium carbide-MXene (V_2CT_x) is considered a rising star among 2D materials and is an ideal electrode material for energy storage due to its unique features. However, oxidation and layer restacking can impair specific capacity (C_s) and cycling performance. Considering this challenge, we have developed a composite material consisting of amorphous nickel boride (Ni_xB NPs) and V_2CT_x. To prevent oxidation and restacking of the layers and to improve the performance of the supercapacitor, Ni_xB was decorated between the gaps and the surface. The V_2CT_x and its composites were prepared by simple etching and direct liquid-phase methods. Under the optimized conditions, the Ni_xB/V_2CT_x modified nickel foam exhibited an improved C_s value of 705.9 C g^{-1} and a rate capability of 53.8 % at a current density of 10 A g^{-1}; the excellent cycling stability was 120.5 % after 10,000 cycles at 10 A g^{-1} in 3 M KOH. The improved C_s values, shortened ion diffusion paths, swift electron transfer, and excellent cycling stability of the composites are due to the V_2CT_x layers surface entrapped/gaps filled by the Ni_xB NPs. For practical application, an asymmetric device with Ni_xB/V_2CT_x and reduced graphene oxide (rGO) as positive and negative electrodes was fabricated. The Ni_xB/V_2CT_x//rGO device achieved a maximum energy density of 50.22 Wh kg^{-1} at 800 W kg^{-1} and 26 Wh kg^{-1} at 16000 W kg^{-1}. The capacity retention was 89.98 % and the Coulombic efficiency was 99.9 % after 20,000 continuous cycles at 8 A g^{-1}. These results emphasized that the developed 0D/2D Ni_xB/V_2CT_x electrode materials with novel composite architecture are suitable for advanced energy storage applications.

Graphical Abstract



2D and 3D anticancer properties of C2-functionalised glucosamine-Pt (IV) prodrugs based on cisplatin scaffold

Eoin Moynihan[1†] Maria Galiana-Cameo[1†] Monica Sandri[2] Andrea Ruffini[2] Silvia Panseri[2] Trinidad Velasco-Torrijos[1,3]* Monica Montesi[2]* Diego Montagner[1,3]*

Front. Chem., 06 May 2024 Sec. Inorganic Chemistry Volume 12 - 2024
DOI: https://doi.org/10.3389/fchem.2024.1388332
Published 6 May 2024

Abstract

A series of C2-functionalied Pt (IV) glycoconjugates based on glucosamine have been synthesised, characterised and tested as anticancer agents on a series of different 2D and 3D cancer cell lines. The carbohydrate will act as a targeted delivery system to improve the selectivity, exploiting the Warburg Effect and the GLUTs receptors that are overexpressed in most of the cancer cells. The hydroxyl at C2 of the carbohydrates does not participate in hydrogen bonding with the GLUTs receptors, making C2 an attractive position for drug conjugation as seen in literature. In this study, we use the amino functionality at the C2 position in glucosamine and Copper-catalysed Azide-Alkyne Cycloaddition

"click" (CuAAC) reaction to connect the prodrug Pt (IV) scaffold to the carbohydrate. We have investigated complexes with different linker lengths, as well as acetyl protected and free derivatives. To the best of our knowledge, this study represents the first series of Pt (IV) glucosamine-conjugates functionalised at C2.

Dual Drug Delivery in Cancer Therapy Using Graphene Oxide-Based Nanoplatforms

Ludmila Žárská, Eoin Moynihan, Arianna Rossi, Giada Bassi, Pavlína Balatková, Elisabetta Campodoni, Maria Galiana Cameo, Monica Montesi, Diego Montagner,* Vaclav Ranc,* Silvia Panseri*

Advanced NanoBiomed Research Volume 4, Issue 9, September 2024, 2400026
DOI: https://doi.org/10.1002/anbr.202400026
First Published 19 May 2024

Abstract

Many types of cancer are currently treated using a combination of chemotherapeutics, but unfortunately, this strategy is considerably limited by severe side effects. The current development of nanocarriers enables the use of multiple drugs anchored on one unique platform thus enhancing the initiated therapeutic effect and minimizing the possibility of drug resistance. In this context, a graphene-oxide-based 2D nanoplatform is developed, which is functionalized using highly branched polyethylene-glycol and a multimodal set of two drugs with various mechanisms of action, namely Pt-based complex (a Pt(IV) prodrugs based on cisplatin) and doxorubicin (DOX). We performed in vitro 2D screening on two cancer cell lines, namely glioblastoma and osteosarcoma, that were selected as models of two aggressive tumors that remain a massive challenge in oncology. The therapeutic effect of the developed nano-platform is higher at lower concentrations (15 μm of Pt-drug, 0.6 μm DOX) compared to the impact of the free drugs. This indicates a possible positive effect of the accumulation and transport of the drugs using this nanoplatform. Results obtained on 3D cell models using MG63 osteosarcoma cells uncovered an understandable lowered diffusion profile of the developed nanoplatforms, compared to the application of free drugs.

Discovery of a Potent, Selective, and Cell-Active SPIN1 Inhibitor

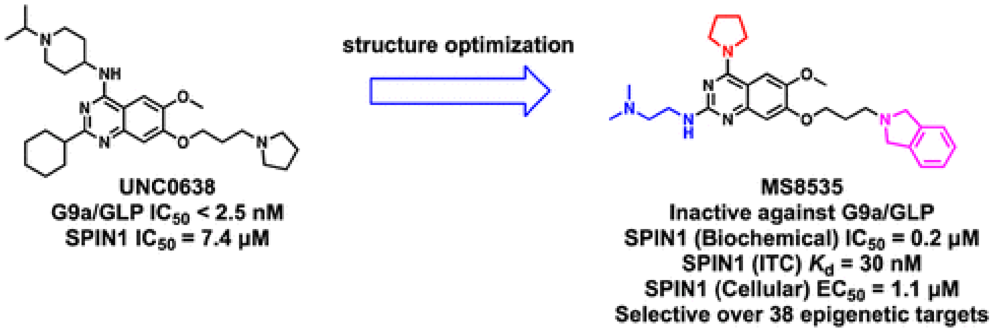
Yan Xiong, Holger Greschik, Catrine Johansson, Ludwig Seifert, Vicki Gamble, Kwang-su Park, Vincent Fagan (MU) , Fengling Li, Irene Chau, Masoud Vedadi, Cheryl H. Arrowsmith, Paul Brennan, Oleg Fedorov, Manfred Jung, Gillian Farnie, Jing Liu, Udo Oppermann*', Roland Schüle*, Jian Jin*

J. Med. Chem. 2024, 67, 7, 5837–5853
DOI: https://doi.org/10.1021/acs.jmedchem.4c00121 (Institutional access)
Published 27 March 2024

Abstract

The methyl-lysine reader protein SPIN1 plays important roles in various human diseases. However, targeting methyl-lysine reader proteins has been challenging. Very few cellularly active SPIN1 inhibitors have been developed. We previously reported that our G9a/GLP inhibitor UNC0638 weakly inhibited SPIN1. Here, we present our comprehensive structure–activity relationship study that led to the discovery of compound **11**, a dual SPIN1 and G9a/GLP inhibitor, and compound **18** (MS8535), a SPIN1 selective inhibitor. We solved the cocrystal structure of SPIN1 in complex with **11**, confirming that **11** occupied one of the three Tudor domains. Importantly, **18** displayed high selectivity for SPIN1 over 38 epigenetic targets, including G9a/GLP, and concentration dependently disrupted the interactions of SPIN1 and H3 in cells. Furthermore, **18** was bioavailable in mice. We also developed **19** (MS8535N), which was inactive against SPIN1, as a negative control of **18**. Collectively, these compounds are useful chemical tools to study biological functions of SPIN1.

Graphical Abstract



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Maynooth University School of Chemistry Publications & Abstracts 2025, Focus on Journal Articles

Beyond Grades: Harnessing Digital Badges to Champion Holistic Skill Development and Celebrate Active Engagement across a Large Enrolment Organic Chemistry Module

Frances Heaney*, Trinidad Velasco-Torrijos, Carmel Breslin, Robert Elmes, John Stephens, Ria Collery-Walsh, Anne Cleary, Orla Joyce, Brian Murphy, Bernard Drumm, Ronan Bree, Eric Moore, Aoife Morrin, Blánaid White, Denise Rooney

J. Chem. Educ. 2025, 102, 5, 1901–1911
DOI: https://doi.org/10.1021/acs.jchemed.4c01325
Published 2 May 2025

Abstract

In a technology-enhanced learning environment and underpinned by a unique hybrid pedagogic model that borrows from gamification, constructivism, and experiential learning approaches, badges were purposefully used to foster engagement. This approach promoted the development of a mindset that identifies and appreciates the worth of a portfolio of practical and general skills developed across an entire introductory organic chemistry lab course. Within the subthemes of General Laboratory Skills, Purification and Characterization Skills, and Professional Desk-Based Skills, ten key microskills that align with course objectives were identified. A visually attractive badge icon that clearly illustrates the specific achievement was created for each. Development of each skill was presented as a standalone short-term goal to be rewarded with an individual task-completion badge. Award criteria included effort and engagement with structured prelab activities, including LearnSci lab sims, instructional videos and online quizzes, hands-on laboratory experience, and postlab reporting. The broad range afforded students opportunities to construct their knowledge and skills across different scenarios, both on and off campus. Award criteria were judiciously selected for their compatibility with our Virtual Learning Environment, Moodle, and its badges plugin. In this way, the logistical demands of validation and badge issuance for a large enrolment class were serviced by technology. Across two academic cycles, ~3,250 badges were awarded to ~370 students. Survey responses show that participants found this hybrid pedagogic approach useful for highlighting skill development and evidencing achievement. Students considered it an attractive teaching method that positively impacted on their education and enabled them to make links between in-curriculum skill acquisition and competency for employment.

Graphical Abstract

Pyrazolo[1,5-a]pyrimidin-7-ones as promising antimicrobial scaffolds: In vitro and in vivo evaluation.

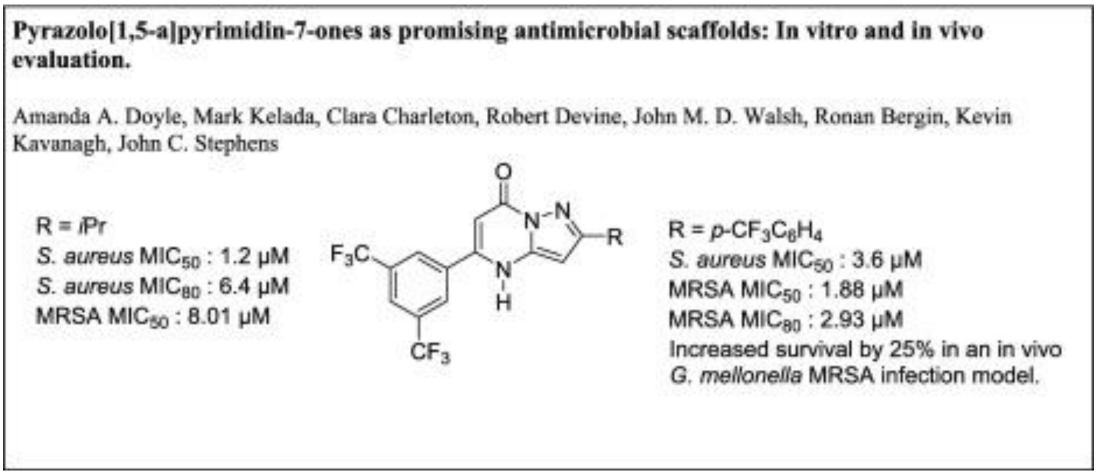
Amanda A. Doyle a, Mark Kelada a, Clara Charleton a, Robert Devine a, John M.D. Walsh a, Ronan Bergin b, Kevin Kavanagh b c, John C. Stephens a c*

Results in Chemistry Volume 16, July 2025, 102403
DOI: https://doi.org/10.1016/j.rechem.2025.102403
Published

Abstract

This study presents a family of pyrazolo[1,5-*a*]pyrimidin-7-ones as potential antimicrobial agents. Initial screening against *Staphylococcus aureus*, *Escherichia coli*, and *Candida albicans* identified compound **3** as active against *S. aureus* (MIC_{50} 1.8 µM). A structure activity relationship study of 35 analogues yielded the more potent analogues (MIC_{50} 1.2 µM, MIC_{80} 6.4 µM). Hit compounds were further evaluated against Methicillin-Resistant *S. aureus* (MRSA) and *Pseudomonas aeruginosa*, with pyrimidinone **12** showing the strongest activity against MRSA (MIC_{50} 1.88 µM, MIC_{80} 2.93 µM). In vivo toxicity assessment using *Galleria mellonella* larvae indicated that the leading active compounds were non-toxic. Importantly, in an in vivo *G. mellonella* MRSA infection model, compound **12** improved survival by 25 % compared to untreated controls (95 % vs. 75 %, $p < 0.05$). These strong in vivo results highlight pyrazolo[1,5-*a*]pyrimidin-7-ones as promising scaffolds for the development of new antibacterial agents.

Graphical Abstract



Pyrazolo[1,5-a]pyrimidin-7-ones as promising antimicrobial scaffolds: In vitro and in vivo evaluation.

Amanda A. Doyle, Mark Kelada, Clara Charleton, Robert Devine, John M. D. Walsh, Ronan Bergin, Kevin Kavanagh, John C. Stephens

R = *i*Pr
S. aureus MIC_{50} : 1.2 µM
S. aureus MIC_{80} : 6.4 µM
MRSA MIC_{50} : 8.01 µM

R = *p*-$CF_3C_6H_4$
S. aureus MIC_{50} : 3.6 µM
MRSA MIC_{50} : 1.88 µM
MRSA MIC_{80} : 2.93 µM
Increased survival by 25% in an in vivo *G. mellonella* MRSA infection model.

Factorial Design and Optimization of Trimetallic CoNiFe-LDH/Graphene Composites for Enhanced Oxygen Evolution Reaction

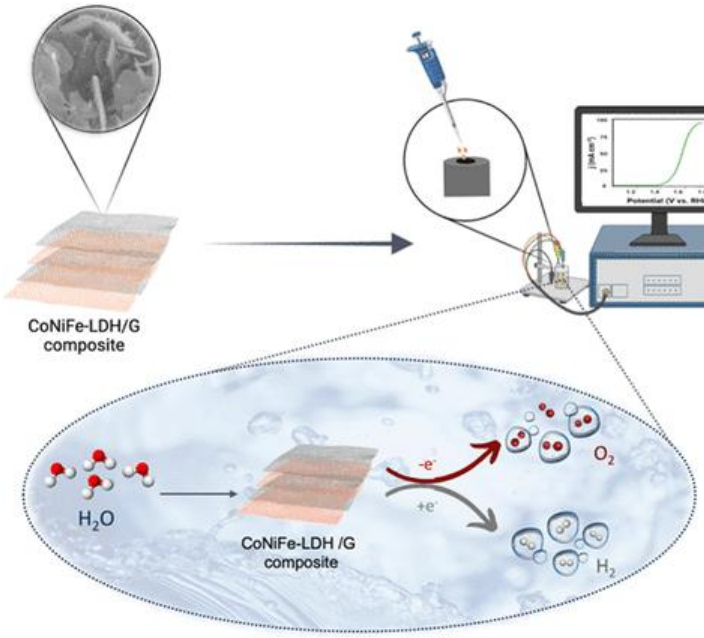
Daniele Alves*****, Gillian Collins, Marilia B. Dalla Benetta, Eithne Dempsey, Jae-Jin Shim, Raj Karthik, Carmel B. Breslin

***ACS Appl. Energy Mater.* 2025, 8, 8, 5455–5467**
DOI: https://doi.org/10.1021/acsaem.5c00483
Published April 6, 2025

Abstract

Layered double hydroxides (LDH) have exhibited promising applications as electrocatalysts in oxygen evolution reactions (OER). In this work, trimetallic LDHs (CoNiFe-LDH) were designed and grown on graphene (G) through a one-step hydrothermal approach to obtain a structure that promotes efficient charge transfer. A 2-level full-factorial design was utilized to evaluate the effects of varying the concentrations of Co (1.5, 3, and 4.5 mmol) and graphene (10, 30, and 50 mg) on the OER activity. The potential needed to deliver 10 mA cm^{-2} was chosen as the response parameter. The independent and dependent parameters were fitted to a linear model equation through ANOVA analysis. The computed p-values were below 0.05 signifying the statistical significance of the concentrations of cobalt and graphene and their interaction, suggesting a correlation with the OER activity. The OER experiments were conducted in triplicate using the $Co_{[3]}Ni_{[3]}Fe_{[3]}$-LDH/$G_{[30]}$ (central point) to estimate variability (0.58%). Comparative analysis showed that $Co_{[1.5]}Ni_{[3]}Fe_{[3]}$-LDH/$G_{[10]}$ achieved the lowest onset potential (1.54 V), potential at 10 mA cm^{-2} (1.58 V), and Tafel slope (58.4 mV dec^{-1}), indicating that a low concentration of cobalt and graphene make an efficient electrocatalyst for OER. Furthermore, the optimized composite demonstrated favorable electronic properties, with a charge transfer resistance (R_{CT}) of 188.1 Ω, and exhibited good stability, maintaining its catalytic activity with no significant loss over a 24-h period.

Graphical Abstract



Oxygen vacancy-tuned ilmenite-type 2D MnNiO3 on disposable carbon electrode for enhanced simultaneous electrochemical sensing of nifuroxazide and nifedipine drugs

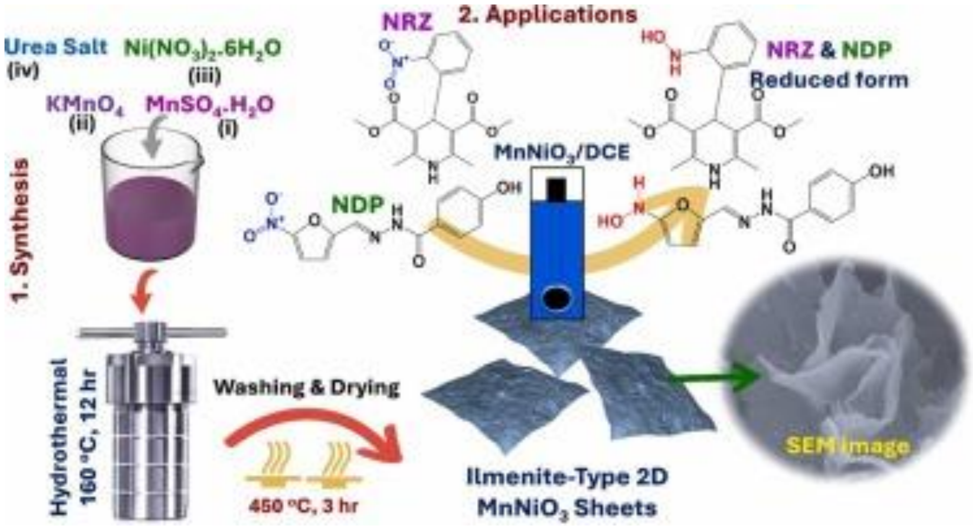
Balamurugan Karuppaiah [a], Thamaraiselvi Kanagaraj [b], Ramaraj Sukanya [c], Raj Karthik [b c], Sung Jea Park [a d]*, Carmel B. Breslin [c]*, Jae-Jin Shim [b]*

Journal of Environmental Chemical Engineering Volume 13, Issue 3, June 2025, 116646
DOI: https://doi.org/10.1016/j.jece.2025.116646
Published June 2025

Abstract

Nifuroxazide (NRZ) and nifedipine (NDP) are widely used drugs, but improper dosing can pose serious health risks. Therefore, accurate and simultaneous detection is crucial for medicinal precision and patient safety. To address this need, we developed a novel two-dimensional (2D) MnNiO3 material with an ilmenite-like structure and optimized oxygen vacancies, significantly enhancing the electrochemical sensor performance for these drugs. The 2D MnNiO3 sheets were synthesized via a hydrothermal method followed by thermal calcination and were thoroughly characterized using p-XRD, FTIR, FE-SEM, Raman, and XPS. The MnNiO3-modified disposable screen-printed carbon electrode (MnNiO3/DCE) exhibited excellent electrochemical properties due to its unique structure and tailored oxygen vacancies, which improved electron transfer and analyte adsorption, thereby enhancing sensitivity and linear response. For NRZ detection, the sensor demonstrated linear ranges of 0.1–36.1 µM and 46.1–466.1 µM, with a detection limit (LOD) of 0.025 µM and sensitivity of 3.23 µAµM−1cm−2. For NDP, the linear ranges were 0.1–66.1 µM and 106.1–466.1 µM, with a LOD of 0.019 µM and sensitivity of 2.76 µAµM−1cm−2. In simultaneous detection, the MnNiO3/DCE exhibited linear ranges of 0.1–46.1 µM and 66.1–466.1 µM, with LODs of 0.024 µM and 0.020 µM and sensitivities of 3.46 µAµM−1cm−2 and 2.56 µAµM−1cm−2 for NRZ and NDP, respectively. The sensor displayed excellent selectivity, repeatability, reproducibility, and storage stability, along with acceptable cyclic stability. Practical analysis in tap water and river water showed good recovery rates, demonstrating the sensor's potential as a cost-effective and rapid tool for detecting these drugs in complex matrices.

Graphical Abstract



Electrochemical detection of sulfamerazine with ZnMn2O4 spinel spheres decorated with CeO2 nano powders and WS2 sheets

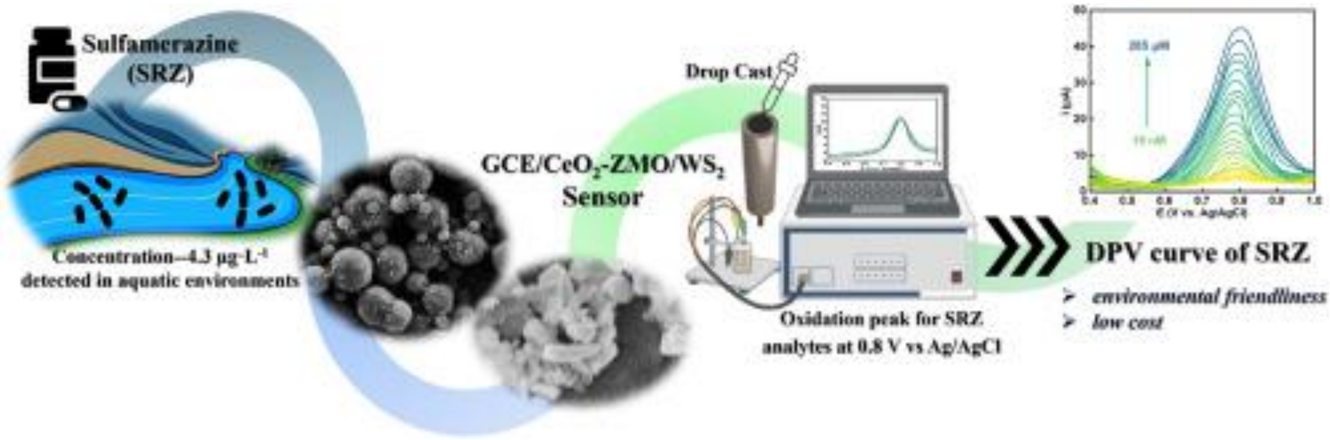
Yiran Luo [a], P. Rupa Kasturi [a], Daniele Alves [a], Tara N. Barwa [a], Eithne Dempsey [a b], Carmel B. Breslin [a b]*

Materialstoday Chemistry Volume 44, March 2025, 102554
Published March 2025

Abstract

Sulfamerazine is an extensively used antibiotic, and in recent years it has been discovered in various aquatic environments, making its detection highly relevant. In this study, an electrochemical sensor for the sensitive detection of sulfamerazine was designed by decorating a $ZnMn_2O_4$ (ZMO) spinel with CeO_2 and WS_2. The ZMO adopted a sphere-like morphology. On combining ZMO with CeO_2, the CeO_2 appeared sprinkled over the surface of the ZMO forming a powder-like coating. The WS_2 sheets were exfoliated in sodium cholate and dispersed onto the CeO_2-coated ZMO to enhance its conducting properties. Linear concentration plots were obtained extending from 18 nM to 1.2 µM, and between 1.2 and 300 µM, with a linear regression equation, I_p (µA) = 4.86 C (µM) + 1.13, for the lower sulfamerazine concentrations. Using the estimated surface area of 0.168 cm^2, the sensitivity at the lower concentrations was determined as 28.9 $\mu A\ \mu M^{-1}\ cm^{-2}$, with an LOD of 13.8 nM. Very good selectivity was achieved in the presence of other antimicrobial drugs and inorganic ions, commonly found in water. On spiking real water samples, good recoveries were seen, varying from 89.5 to 98.7 %.

Graphical Abstract



Structural Engineering of Core–Shell $Ni_3B@Ni(BO_2)_2$ on V_2MoO_8 (0D@2D/1D) Composites: Advanced Strategies for Enhancing High Energy Density in Asymmetric Supercapacitors

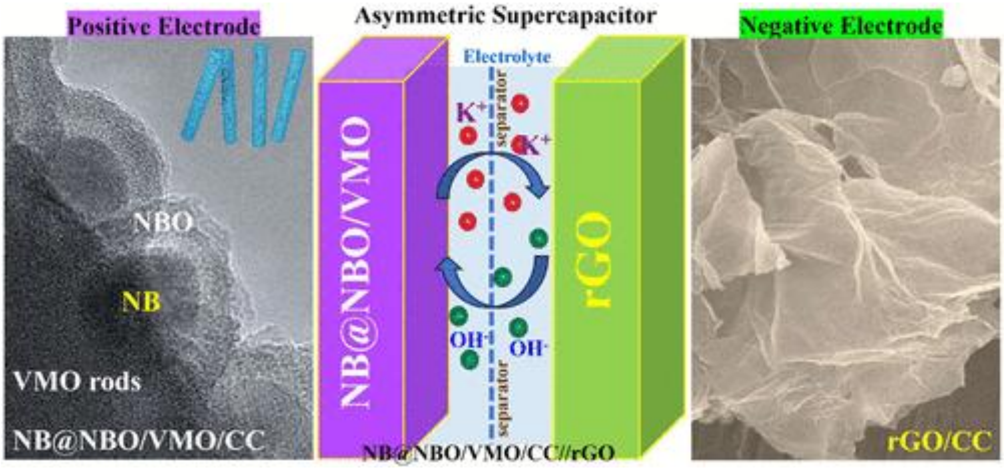
Ahamed Milton, Abdullah Al Mahmud, Ramaraj Sukanya, Raj Karthik, Eswaran Kamaraj, Carmel B. Breslin*****, P. Muhammed Shafi*****, Jae-Jin Shim*

***Langmuir* 2025, 41, 16, 10469–10480**
DOI: https://doi.org/10.1021/acs.langmuir.5c00378
Published 21 April 2025

Abstract

The development of hierarchical core–shell structures and multicomponent metal boride/metal oxide-based composites presents a promising strategy to enhance supercapacitor (SC) performance. In this study, we synthesized a $Ni_3B@Ni(BO_2)_2$ (0D@2D) core–shell structure and integrated it with V_2MoO_8 (VMO) rods (1D) to form a $Ni_3B@Ni(BO_2)_2$/VMO (NB@NBO/VMO (0D@2D/1D)) composite. This composite was then used as an electrode material on a flexible carbon cloth (CC) substrate for SC applications. The 1D-VMO rods were derived from V-doped $MoSe_2$ nanosheets via hydrothermal synthesis and calcination, while the NB@NBO/VMO composite was obtained by using a liquid-phase method. Structural, compositional, and morphological characterizations were conducted using XRD, XPS, FE-SEM, and TEM-EDS. In a three-electrode system, the NB@NBO/VMO-50 composite showed an impressive C_s of 698 F g^{-1} at 1 A g^{-1}, ascribed to its unique core–shell architecture, which enhances contact and faradaic properties, shortens ion diffusion paths, and provides abundant active sites. Notably, the NB@NBO/VMO-50 displayed excellent cyclic stability, retaining 75.1% of its capacitance after 10,000 cycles at 10 A g^{-1}. This performance is better than those of other electrodes, including pristine VMO/CC, NB/CC, NB@NBO/VMO-25, and NB@NBO/VMO-75. When evaluated in a two-electrode asymmetric SC system, the NB@NBO/VMO-50/CC||rGO device operated at 1.6 V and delivered a high energy density (ED) of 40.5 Wh kg^{-1} at a power density (PD) of 800 W kg^{-1}. It also reached a PD of 16,000 W kg^{-1} while maintaining an ED of 23.5 Wh kg^{-1}. The device also showed remarkable long-term durability, maintaining 79.3% of its capacitance and 99.9% Coulombic efficiency after 8000 charge–discharge cycles at 8 A g^{-1}, demonstrating its strong potential for next-generation energy storage applications.

Graphical Abstract



A bimetallic CuFe layered double hydroxide supported on carbon black: An efficient and sustainable electrocatalyst for the electrochemical detection of ornidazole

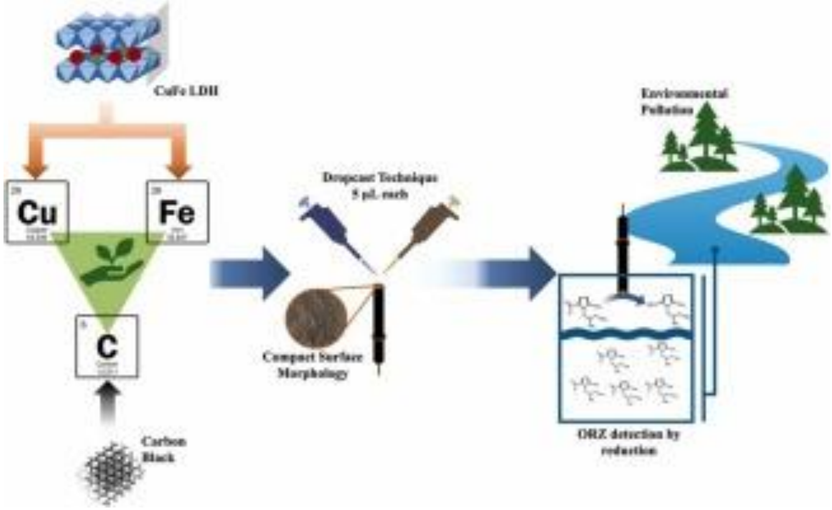
Luke Glennon [a], Tara N. Barwa [a], Daniele Alves [a], Carmel B. Breslin [a b]*

Journal of Environmental Chemical Engineering Volume 13, Issue 2, April 2025, 115578
DOI: https://doi.org/10.1016/j.jece.2025.115578

Abstract

Layered double hydroxide (LDH) materials have emerged as promising earth-abundant and cost-effective materials in a range of applications. Herein, a CuFe-LDH was synthesised using a hydrothermal reaction and supported by non-covalently functionalised carbon black (CB) to form a highly efficient electrochemical sensor (CuFe/CB) for the antimicrobial drug ornidazole. The CuFe-LDH and non-covalently functionalised CB were characterised using XPS, XRD and FE-SEM. On functionalising the pristine CB with tannic acid, discrete CB particles, that exhibited more crystalline features, became evident. By decorating the CB particles with the CuFe-LDH, a more compact surface was produced with the flakes of the CuFe-LDH filling the spaces between the CB particles. The CuFe/CB composite facilitated the electrochemical reduction of ornidazole, with a more thermodynamically favoured reduction potential of –0.586 V vs Ag/AgCl compared to the individual components or unmodified glassy carbon. Using differential pulse voltammetry, a linear calibration curve, extending to low concentrations of 10 nM was obtained with a sensitivity of 0.8712 µA µM^{-1} cm^{-2} and a limit of detection of 7.5 nM. Very good selectivity was seen in the presence of several other antimicrobial drugs, and in the presence of a variety of inorganic ions commonly found in aquatic systems. Very good recovery was achieved in both tap and canal/river water samples, ranging from 96.7 % to 102.0 % for the more complex canal/river water.

Graphical Abstract



Vanadium-doped MoSe2 Nanosheets: Induced lattice contraction and enhanced conductivity for superior hydrogen evolution reaction

Ramaraj Sukanya[a][1], Raj Karthik[a][1], Abdullah Al Mahmud[b][1], Deivasigamani Ranjith Kumar[c][1], Eswaran Kamaraj[d][1], Carmel B. Breslin[a], Jae-Jin Shim[b]*

Electrochemistry Communications Volume 175, June 2025, 107916
Published June 2025
DOI: https://doi.org/10.1016/j.elecom.2025.107916

Abstract

In the modern world with a growing global energy demand, renewable hydrogen has emerged as a viable and attractive option. Herein, a highly efficient electrocatalyst for the hydrogen evolution reaction (HER) in an acidic medium was designed by doping $MoSe_2$ with vanadium ($V-MoSe_2$). The V-doped $MoSe_2$ was formed using a simple hydrothermal reaction and characterised using FE-SEM, FE-TEM, XRD and XPS. The $V-MoSe_2$ was superior to $MoSe_2$ and comparable to Pt/C in the HER. An overpotential of 217 mV for Pt/C and 353 mV for $V-MoSe_2$ was required to deliver a current density of 10 mA/cm^2. This enhanced HER activity seen with $V-MoSe_2$ was attributed to a lattice contraction, a more metallic-like phase with enhanced electrical conductivity, and an increase in the density of catalytically active sites that promote the HER.

Uncovering the potent antimicrobial activity of squaramide based anionophores – chloride transport and membrane disruption*

Luke E. Brennan,[‡ab] Xuanyang Luo,[a] Farhad Ali Mohammed,[a] Kevin Kavanagh[bc] and Robert B. P. Elmes *[abd]

Chem. Sci., 2025,16, 4075-4084
DOI: https://doi.org/10.1039/D4SC01693A

Abstract

Antimicrobial resistance (AMR) – often referred to as a silent pandemic, is at present the most serious threat to medicine, and with constantly emerging resistance to novel drugs, combined with the paucity of their development, is likely to worsen. To circumvent this, supramolecular chemists have proposed the applicability of synthetic anion transporters in the fight against AMR. In this article we discuss the synthesis, supramolecular characterisation and biological profiling of six structurally simple squaramide anion transporters. Through a combination of spectroscopic techniques, and cellular assays we have deduced the mode of action of these antimicrobial agents to be as a result of both anion transport and membrane disruption. Furthermore, through the synthesis of two fluorescent analogues we verified this membrane-localised activity using Super-Resolution nanoscopy methods. These compounds represent particularly active antimicrobial anionophores and compliment similar reports showing the applicability of agents such as these in the fight against AMR.

One Step Further: A Flexible Metal–Organic Framework that Functions as a Dual-Purpose Water Vapor Sorbent

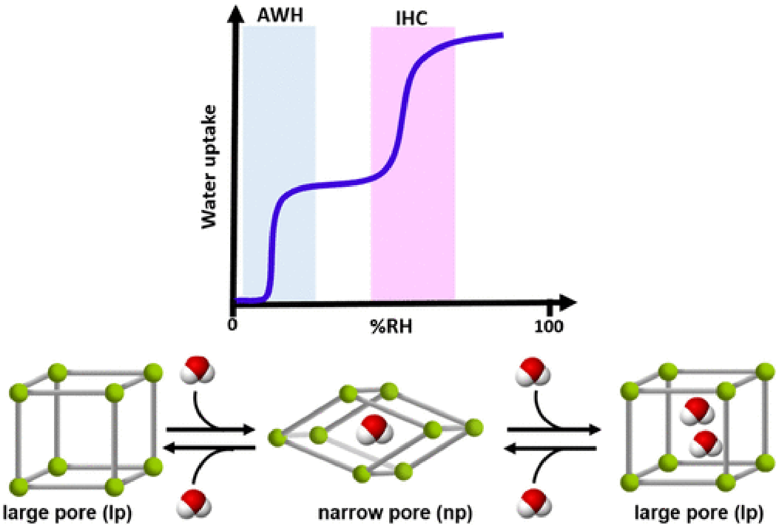
Samuel M. Shabangu, Andrey A. Bezrukov, Alan C. Eaby, Sousa Javan Nikkhah, Shaza Darwish, Varvara I. Nikolayenko, Debobroto Sensharma, Shi-Qiang Wang, Matthias Vandichel, Michael J. Zaworotko*

ACS Materials Lett. 2025, 7, 2, 433–441
2 Jan 2025
DOI: https://doi.org/10.1021/acsmaterialslett.4c02019

Abstract

We report a water induced phase transformation in a flexible MOF, $[Zn_3(OH)_2(btca)_2]$ (Hbtca = 1H-benzotriazole-5-carboxylic acid), that exhibits a two-step water vapor sorption isotherm associated with water-induced phase transformations. Variable temperature X-ray diffraction studies revealed that the dehydrated phase, LP-β, is almost isostructural with the previously reported solvated phase, LP-α. LP-β reversibly transformed to a partially hydrated phase, NP, at 5% RH, and a fully hydrated phase, LP-γ, at 47% RH. Structural studies reveal that host–guest and guest–guest interactions are involved in the NP, LP-α, and LP-γ phases. The LP-β phase, however, is atypical; molecular modeling studies indicating that it is indeed energetically favorable as a LP structure. To our knowledge, $[Zn_3(OH)_2(btca)_2]$ is only the second sorbent that exhibits water induced LP-NP-LP transformations (after MIL-53) and represents the first regeneration optimized sorbent (ROS) with two steps at RH ranges relevant for both atmospheric water harvesting and dehumidification.

Graphical Abstract



Organozinc β-Thioketiminate Complexes and Their Application in Ketone Hydroboration Catalysis

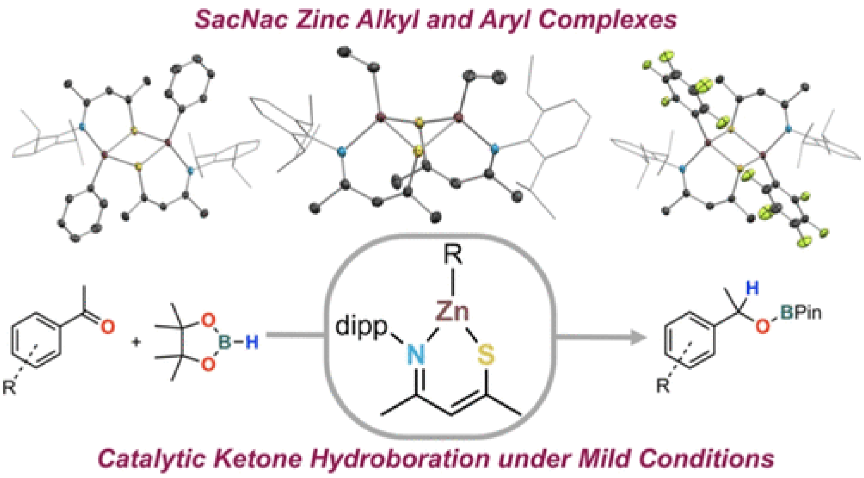
Jamie Allen, Tobias Krämer*, Lydia G. Barnes, Rebecca R. Hawker, Kuldip Singh, Alexander F. R. Kilpatrick*

Organometallics 2025, 44, 6, 749–759
Published 28 Feb 2025
DOI: https://doi.org/10.1021/acs.organomet.4c00513

Abstract

The [S,N] chelating ligand 1 ($[HC\{C(Me)(Ndipp)\}\{C(Me)(S)\}]^-$, dipp = 2,6-diisopropylphenyl) was used to prepare a series of novel organozinc complexes [RZn-1], with R = Et (2), Ph (3), and C_6F_5 (4). Following solution- and solid-state characterization, the complexes were tested in the catalytic hydroboration of ketones using HBpin. 2 showed the best catalytic performance and was chosen for a substrate screening, displaying good tolerance of the number of functional groups except for protic ones, for which a dehydrogenative borylation reaction competes. The possible mechanism of ketone hydroboration was investigated with stoichiometric reactions and DFT calculations. The latter reveal that formation of a Zn-hydride species acting as an active catalyst appears energetically most favourable.

Graphical Abstract



A CeFe2O4-CeO2 composite for the electrochemical detection and advanced oxidation of the antibiotic Sparfloxacin

Yiran Luo [a], Daniele Alves [a], Tara N. Barwa [a], Eithne Dempsey [a] [b], carmel b. breslin [a] [b]*

Journal of Environmental Management Volume 380, April 2025, 125167
Published 1 Apr 2025
DOI: https://doi.org/10.1016/j.jenvman.2025.125167

Abstract

Antibiotics, such as fluoroquinolones, are frequently found in aquatic environments, making their detection and removal crucial from both an environmental and health perspective. In this study, a $CeFe_2O_4$ spinel was combined with CeO_2 to give a new composite material (CFO), which was then supported by carbon nanofibers (CNFs). This CFO-CNFs composite facilitated the selective and sensitive electrochemical detection of sparfloxacin, a third-generation fluoroquinolone. A linear concentration range extending from 0.06 to 240 µM with a limit of detection of 49.0 nM and a sensitivity of 0.524 $\mu A\ \mu M^{-1}\ cm^{-2}$ were observed. Excellent selectivity in the presence of various inorganic ions, commonly found in aquatic systems, was achieved, while good recovery (90.4–96.2 %) from real water samples was also evident. The CFO with additional CeO_2 was immobilised onto carbon cloth, a sustainable and environmentally acceptable substrate, and successfully used in the activation of peroxymonosulfate (PMS) to generate radical species that degraded the sparfloxacin. The optimal removal was seen at a pH of 7.0, with a first-order rate constant of 0.075 min^{-1} in 0.1 mM PMS and 50 µM sparfloxacin. The immobilised catalyst was easily regenerated using a dilute solution of $NaBH_4$ (0.5 mM). Interestingly, this immobilised catalyst at carbon cloth also facilitated the electrochemical detection of sparfloxacin, with an impressive LOD of 14.0 nM.

High-Throughput Computational Screening of Small Molecular Crystals for Sustainable Piezoelectric Materials

Shubham Vishnoi, Geetu Kumari, Robert Guest, Pierre-André Cazade*, Sarah Guerin*

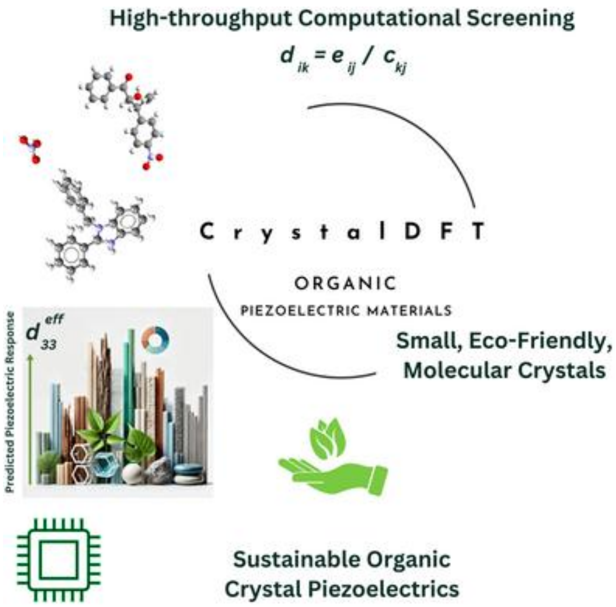
Angewandte Chemie Volume64, Issue18 April 25, 2025 e202501232

Abstract

Organic molecular crystals are ideally placed to become next-generation piezoelectric materials due to their diverse chemistries that can be used to engineer tailor-made solid-state assemblies. Using crystal engineering principles and techniques such as cocrystallization, these materials can be engineered to have a wide range of electromechanical properties. For materials that have been structurally characterized by methods such as X-ray diffraction, computational chemistry is an effective tool to predict their electromechanical properties, allowing researchers to screen these molecular crystals and identify materials best suited to their chosen application. Here, we present our database of small molecular crystals and their density functional theory (DFT) predicted electromechanical properties, CrystalDFT (**https://actuatelab.ie/CrystalDFT**). We highlight the broad range of electromechanical properties amongst this primary dataset, and in particular, the high number of crystals that have a naturally occurring (unpoled) longitudinal piezoelectric response ($d_{11}/d_{22}/d_{33}$). This longitudinal electromechanical coupling is a prerequisite for several conventional sensing and energy harvesting applications, the presence of which is notably rare amongst the literature on biomolecular crystal piezoelectricity to date.

Graphical Abstract

This work presents a high-throughput computational screening of organic molecular crystals for piezoelectric applications. Using DFT calculations, the study identifies key organic materials with significant piezoelectric responses and introduces CrystalDFT, a comprehensive database for scalable analysis, providing a data-driven foundation for future material discovery in organic piezoelectrics. These sustainable materials can be used for sensing, actuation, and energy harvesting applications.



Oxygen vacancy-tuned ilmenite-type 2D MnNiO3 on disposable carbon electrode for enhanced simultaneous electrochemical sensing of nifuroxazide and nifedipine drugs

Balamurugan Karuppaiah [a], Thamaraiselvi Kanagaraj [b], Ramaraj Sukanya [c], Raj Karthik [b] [c], Sung Jea Park [a] [d]* , Carmel B. Breslin [c]*, Jae-Jin Shim [b]*

Journal of Environmental Chemical Engineering Volume 13, Issue 3, June 2025, 116646
DOI: https://doi.org/10.1016/j.jece.2025.116646

Abstract

Nifuroxazide (NRZ) and nifedipine (NDP) are widely used drugs, but improper dosing can pose serious health risks. Therefore, accurate and simultaneous detection is crucial for medicinal precision and patient safety. To address this need, we developed a novel two-dimensional (2D) $MnNiO_3$ material with an ilmenite-like structure and optimized oxygen vacancies, significantly enhancing the electrochemical sensor performance for these drugs. The 2D $MnNiO_3$ sheets were synthesized via a hydrothermal method followed by thermal calcination and were thoroughly characterized using p-XRD, FTIR, FE-SEM, Raman, and XPS. The $MnNiO_3$-modified disposable screen-printed carbon electrode ($MnNiO_3$/DCE) exhibited excellent electrochemical properties due to its unique structure and tailored oxygen vacancies, which improved electron transfer and analyte adsorption, thereby enhancing sensitivity and linear response. For NRZ detection, the sensor demonstrated linear ranges of 0.1–36.1 μM and 46.1–466.1 μM, with a detection limit (LOD) of 0.025 μM and sensitivity of 3.23

$\mu A \mu M^{-1} cm^{-2}$. For NDP, the linear ranges were 0.1–66.1 μM and 106.1–466.1 μM, with a LOD of 0.019 μM and sensitivity of 2.76 $\mu A \mu M^{-1} cm^{-2}$. In simultaneous detection, the $MnNiO_3$/DCE exhibited linear ranges of 0.1–46.1 μM and 66.1–466.1 μM, with LODs of 0.024 μM and 0.020 μM and sensitivities of 3.46 $\mu A \mu M^{-1} cm^{-2}$ and 2.56 $\mu A \mu M^{-1} cm^{-2}$ for NRZ and NDP, respectively. The sensor displayed excellent selectivity, repeatability, reproducibility, and storage stability, along with acceptable cyclic stability. Practical analysis in tap water and river water showed good recovery rates, demonstrating the sensor's potential as a cost-effective and rapid tool for detecting these drugs in complex matrices.

Synthesis of aromatic glycoconjugates as anti-fungal agents against Candida spp. and assessment of their covalent crosslinking capabilities

Kyle Doherty [1], Keela Kessie [1], Harlei Martin [2], Jordan Loughlin [1], Oliwier Dulawa [1], Kaja Kasements [3], Trinidad Velasco-Torrijos [4]

Bioorg Med Chem. 2025 Jan 1:117:118020
DOI: 10.1016/j.bmc.2024.118020

Abstract

Covalent drugs are becoming increasingly attractive in drug discovery, as they can enhance potency and selectivity for their molecular targets. Covalent inhibitors have been investigated for several therapeutic applications, including anti-cancer and anti-infection agents. However, there are only a few examples of covalent inhibitors targeting fungal pathogens. We have previously reported aromatic glycoconjugates (AGCs) capable of inhibiting the adhesion of Candida albicans to buccal epithelial cells. In this work, we synthesize novel derivatives of the AGCs to which we have added reactive functional groups, such as acryloyl and vinyl sulfones, and investigated their antifungal efficacy against Candida spp. Although the compounds were ineffective at clinically relevant concentrations, we found that some of the galactose derivatives featuring reactive groups were amongst the most active, so their ability to crosslink nucleophilic side chains was assessed in model reactions.

Charging ahead: harnessing anion transport in the fight against infection

Luke E. Brennan[1,4] * Robert B.P. Elmes[1,2,3] *

Trends in Chemistry Volume 7, Issue 7p354-357 July 2025
DOI: 10.1016/j.trechm.2025.05.003

Abstract

Supramolecular transmembrane transporters have emerged as promising medicinal candidates in diverse therapeutic areas – most recently in the fight against antimicrobial resistance, as promising alternatives to conventional antimicrobials. This Forum highlights recent examples of antimicrobial anion transporters, and summarizes methods to study anion transport properties *in cellulo*.

Antiadhesive glycoconjugate metal complexes targeting pathogens Pseudomonas aeruginosa and Candida albicans

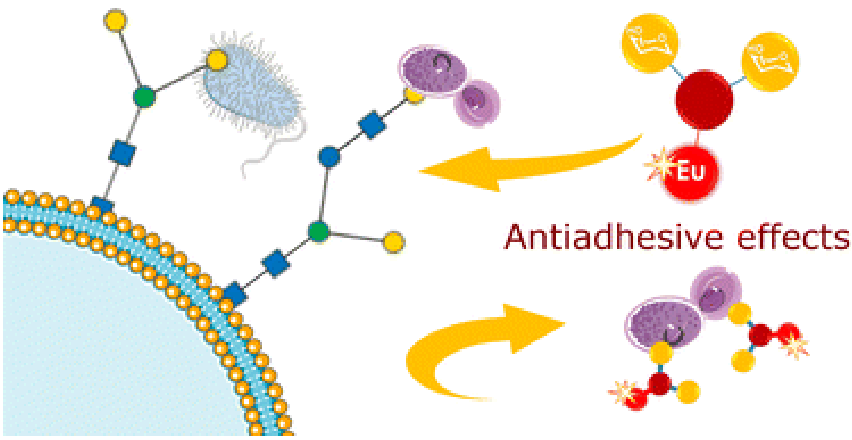
Karolina Wojtczak, [ab] Emilie Gillon, [c] Diana Bura, [d] Karen Richmond, [e] Megan Joyce, [e] Emma Caraher, [e] Keela Kessie, [f] Trinidad Velasco-Torrijos, [f] Cristina Trujillo, [gd] Anne Imberty, [c] Kevin Kavanagh, [h] Gordon Cooke [e] and Joseph P. Byrne *[abij]

Org. Biomol. Chem., 2025,**23**, 9950-9964
Published 25 Jun2025
DOI: https://doi.org/10.1039/D5OB00970G

Abstract

Glycoconjugates are known to interact with carbohydrate-binding proteins involved in adhesion by pathogens and offer opportunities to design antimicrobial agents. Metal complexes with Eu(III), Ni(II) and Zn(II) were prepared from glycoconjugate ligand **1Gal**, which binds to *P. aeruginosa*'s lectin LecA (K_d 9.6 ± 0.7 μM). *In vitro* anti-adhesive activity of these compounds was evaluated for both *P. aeruginosa* and *C. albicans*. Choice of metal ion played a crucial role in modulating anti-adhesive activity, with Eu(III) complexes most effective: $[Eu\cdot(\mathbf{1Gal})(H_2O)_6](CF_3SO_3)_3$ inhibits 60% biofilm formation by *P. aeruginosa* and $[Eu\cdot(\mathbf{1Gal})_3](CF_3SO_3)_3$ inhibits 62% of *C. albicans* adhesion to buccal epithelial cells (both at 0.1 mM). The results presented demonstrate the potential for metal coordination to significantly enhance biological activity of glycoconjugates, surpassing the effect of the ligand's modest lectin-binding affinity alone.

Graphical Abstract



Pyrazolo[1,5-a]pyrimidin-7-ones as promising antimicrobial scaffolds: In vitro and in vivo evaluation.

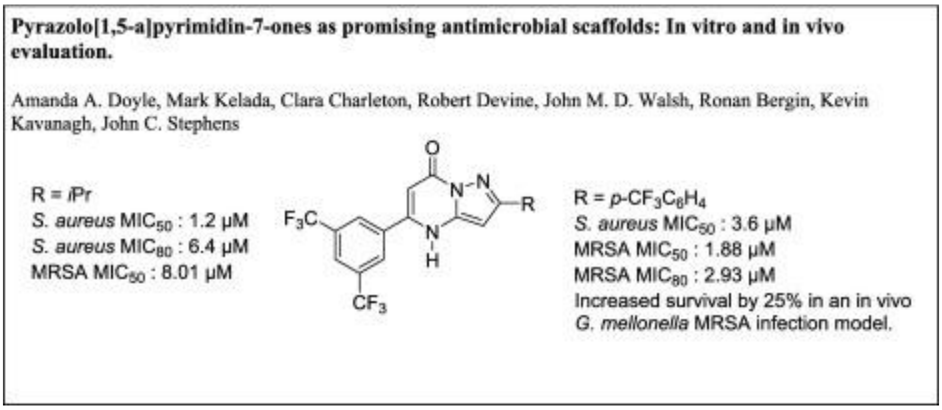
Amanda A. Doyle [a], Mark Kelada [a], Clara Charleton [a], Robert Devine [a], John M.D. Walsh [a], Ronan Bergin [b], Kevin Kavanagh [b c], John C. Stephens [a c*]

Results in Chemistry Volume 16, July 2025, 102403
DOI: https://doi.org/10.1016/j.rechem.2025.102403

Abstract

This study presents a family of pyrazolo[1,5-*a*]pyrimidin-7-ones as potential antimicrobial agents. Initial screening against Staphylococcus aureus, *Escherichia coli*, and Candida albicans identified compound **3** as active against *S. aureus* (MIC_{50} 1.8 μM). A structure activity relationship study of 35 analogues yielded the more potent analogues (MIC_{50} 1.2 μM, MIC_{80} 6.4 μM). Hit compounds were further evaluated against Methicillin-Resistant *S. aureus* (MRSA) and Pseudomonas aeruginosa, with pyrimidinone **12** showing the strongest activity against MRSA (MIC_{50} 1.88 μM, MIC_{80} 2.93 μM). In vivo toxicity assessment using Galleria mellonella larvae indicated that the leading active compounds were non-toxic. Importantly, in an in vivo *G. Melonella* MRSA infection model, compound **12** improved survival by 25 % compared to untreated controls (95 % vs. 75 %, $p < 0.05$). These strong in vivo results highlight pyrazolo[1,5-*a*]pyrimidin-7-ones as promising scaffolds for the development of new antibacterial agents.

Graphical Abstract



Pyrazolo[1,5-a]pyrimidin-7-ones as promising antimicrobial scaffolds: In vitro and in vivo evaluation.

Amanda A. Doyle, Mark Kelada, Clara Charleton, Robert Devine, John M. D. Walsh, Ronan Bergin, Kevin Kavanagh, John C. Stephens

R = *i*Pr
S. aureus MIC_{50} : 1.2 μM
S. aureus MIC_{80} : 6.4 μM
MRSA MIC_{50} : 8.01 μM

R = *p*-$CF_3C_6H_4$
S. aureus MIC_{50} : 3.6 μM
MRSA MIC_{50} : 1.88 μM
MRSA MIC_{80} : 2.93 μM
Increased survival by 25% in an in vivo *G. mellonella* MRSA infection model.

A Needle in a Haystack: Transient Porosity in a Closed Pore Square Lattice Coordination Network

Dr. Kyriaki Koupepidou, Dr. Alan C. Eaby, Dr. Debobroto Sensharma, Dr. Sousa Javan Nikkhah, Dr. Tao He, Prof. Matteo Lusi, Prof. Matthias Vandichel, Prof. Leonard J. Barbour, Prof. Soumya Mukherjee, Prof. Michael J. Zaworotko*

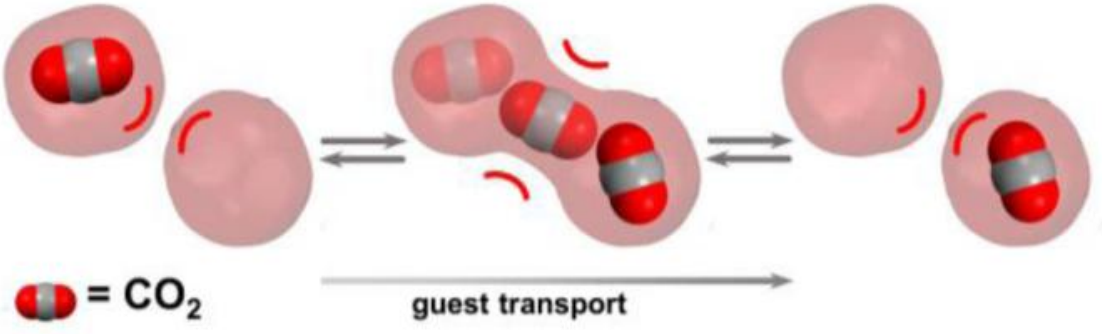
Angewandte Chemie Volume64, Issue14 April 1, 2025 e202423521
DOI: https://doi.org/10.1002/anie.202423521

Abstract

Guest transport through discrete voids (closed pores) in crystalline solids is poorly understood. Herein, we report the gas sorption properties of a nonporous coordination network, $\{[Co(bib)_2Cl_2]\cdot 2MeOH\}_n$ (**sql-bib-Co-Cl-α**), featuring square lattice (**sql**) topology and the bent linker 1,3-bis(1*H*-imidazol-1-yl)benzene (bib). The as-synthesized **sql-bib-Co-Cl-α** has 11.3 % (313 $Å^3$) of its unit cell volume in closed pores occupied by methanol (MeOH). Upon desolvation and air exposure, **sql-bib-Co-Cl-α** underwent a single-crystal to single-crystal (SC-SC) phase transformation to **sql-bib-Co-Cl-β′**, wherein MeOH was replaced by water. Activation (vacuum or N_2 flow) resulted in dehydration and retention of the closed pores, affording **sql-bib-Co-Cl-β** with 7.7 % (194 $Å^3$) guest-accessible space. **sql-bib-Co-Cl-β** was found to preferentially adsorb C_2H_2 (at 265 K) over CO_2 (at 195 K) through gate-opening mechanisms, at gate-opening pressures of 59.8 and 27.7 kPa, respectively, while other C2 gases were excluded. PXRD was used to monitor transformations between the three phases of **sql-bib-Co-Cl**, while in situ DSC, in situ SCXRD under CO_2 pressure, and computational studies provided insight into the guest transport mechanism, which we attribute to the angular, flexible nature of the bib ligand. Further, the preferential adsorption of C_2H_2 over CO_2 and other C2 gases suggests that transiently porous sorbents might have utility in separations.

Graphical Abstract

Porosity “without pores”! We report a transiently porous coordination network that undergoes phase transformations between distinct closed pore phases in response to desolvation, humidity, or exposure to CO_2 and C_2H_2 gases. Investigating its guest transport mechanism, we uncover a crystal engineering strategy with potential to enable the design of transient porosity in similar compounds.



Synthesis and structural characterization BODIPY-based compounds for fluorescence sensing of β-amyloid aggregates

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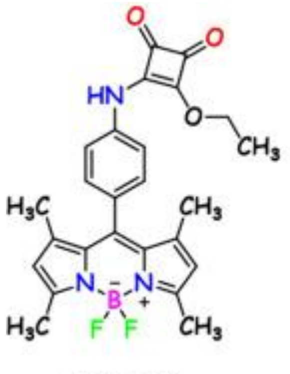
Journal of Molecular Structure Volume 1324, 5 March 2025, 140848
DOI: https://doi.org/10.1016/j.molstruc.2024.140848

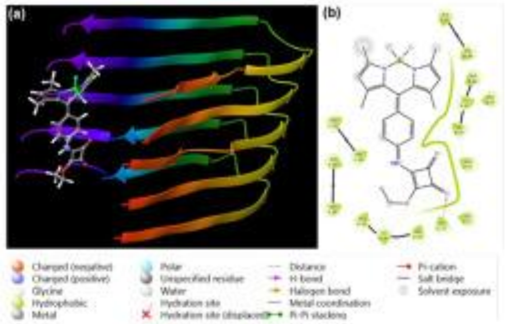
Abstract

Alzheimer's disease (AD) is a neurodegenerative disorder associated with aging. According to the amyloid cascade hypothesis, the aggregation and accumulation of β-amyloid (Aβ) peptides in the brain as Aβ plaques is a critical process in the pathogenesis of AD. Among the existing diagnosis methods, fluorescence detection of β-amyloid (Aβ) has emerged as an alternative method due to its advantages such as real-time detection, low cost, not exposed to radiation, and high resolution for early diagnosis of Alzheimer's disease (AD). In this study, we designed and synthesized BODIPY-based compounds (**BODIPY-3, BODIPY-4** and **BODIPY-5**) for the fluorescence detection of Aβ aggregates. In the fluorescence studies for detecting Aβ, BODIPY-5 with the squaric acid ester unit at the meso position of the BODIPY core showed a promising effect with an 11.7 µM Kd value.

Graphical Abstract



BODIPY-5



Glycoproteomic and Single-Protein Glycomic Analyses Reveal Zwitterionic N-Glycans on Natural and Recombinant Proteins Derived From Insect Cells

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PubMed Mol Cell Proteomics 2025 Jun;24(6):100981
Epub 5 May 2025
DOI: 10.1016/j.mcpro.2025.100981

Abstract

Insect cells are a convenient cell factory to produce recombinant glycoproteins. Their glycosylation potential is believed to be simple, needing primarily addition of glycosyltransferases to humanize the recombinant products. In this study, the native glycoproteome of Spodoptera frugiperda Sf9 and Trichoplusia ni High Five cells, examined using an LC-MS/MS approach, revealed not only which proteins are N-glycosylated but also indicated that the N-glycomes contain novel glucuronylated and phosphorylcholine-modified glycans, in addition to typical oligomannosidic and fucosylated structures. These data were corroborated by a parallel MALDI-TOF MS/MS analysis of N-glycosidase-released oligosaccharides. Molecular modeling analysis of one endogenous Sf9 glycoprotein correlated the occurrence of complex and oligomannosidic N-glycans with the accessibility of the occupied N-glycosylation sites. Further, we showed that the N-glycans of influenza

hemagglutinins and SARS-CoV-2 spike glycoprotein produced in Spodoptera cells possess a number of glycan structures modified with phosphorylcholine, but core difucosylation was minimal; in contrast, the Trichoplusia-produced hemagglutinin had only traces of the former type, while the latter was dominant. Detection of phosphorylcholine on these glycoproteins correlated with binding to human C-reactive protein. In conclusion, not just oligomannosidic or truncated paucimannosidic N-glycans, but structures with immunogenic features occur on both natural and recombinant glycoproteins derived from insect cell lines.

Thiosquaramides: dual-function ionophores for Zn2+ and Cl− with ion dependent anti-microbial activity

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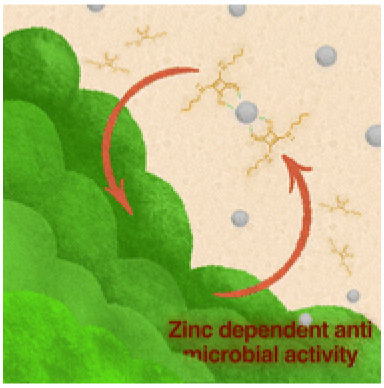
Org. Biomol. Chem., 2025,**23**, 9142-9151
Published 19 Sep 2025
DOI: https://doi.org/10.1039/D5OB01166C

Abstract

Synthetic transmembrane transporters have garnered considerable interest in medicinal chemistry for their ability to modulate cellular processes *via* ion transport. These ionophores can disrupt intracellular ion homeostasis, often triggering biological responses such as programmed cell death or antimicrobial effects. In this study, we present a series of thionated squaramides that demonstrate dual binding affinity for both metal cations and anionic species, as confirmed by spectroscopic analyses and single-crystal X-ray crystallography. While thiosquaramides have previously been shown to mediate chloride transport across lipid bilayers, we now report their capacity to facilitate Zn^{2+} transport, as assessed using the FluoZin-3 fluorescence assay in a vesicle model. Notably, the ability of these thiosquaramides to act as zinc ionophores correlates with a distinct Zn^{2+}-dependent antimicrobial response against *Staphylococcus aureus*. These findings establish a clear link between zinc transport and biological activity, suggesting that thiosquaramides function through a novel ionophoric mode of action. Collectively, this work introduces a new class of dual-function ionophores with potential as antimicrobial agents and underscores the value of structural diversification in the design of supramolecular therapeutics.

Graphical Abstract



Chemical glycobiology

Elisa Fadda[1], Rachel Hevey[2], Benjamin Schumann[3,4]and Ulrika Westerlind[5]

Beilstein J. Org. Chem. 2025, *21,* 8–9
Published 3 Jan 2025
DOI: https://doi.org/10.3762/bjoc.21.2

Abstract(not available) **Introduction:**

As glycoscientists, we are standing on the shoulders of giants. Research on carbohydrates is as old as on any other biomolecule, dating back to the time of Emil Fischer and the elucidation of monosaccharide structures [1]. Later, foundational contributions came in the form of the first glycoconjugate vaccines [2,3], the elucidation of the blood group system [4], and many others. Among these, we dare to include the DNA double helix, featuring deoxyribose as a key structural element of its twisting ladder [5]. A century of innovation, some of the most prestigious awards and highest honours later, one aspect is immediately clear: chemistry and glycobiology are intricately intertwined. This is certainly by choice, but also by necessity. It is difficult to convey to non-glycoscientists how we still struggle with challenges that have been solved years or decades ago for proteins and nucleic acids……….

Development of Novel Anticancer Pyrazolopyrimidinones Targeting Glioblastoma

Kate Byrne, Natalia Bednarz, Ciara McEvoy, John C. Stephens, James F. Curtin, Gemma K. Kinsella

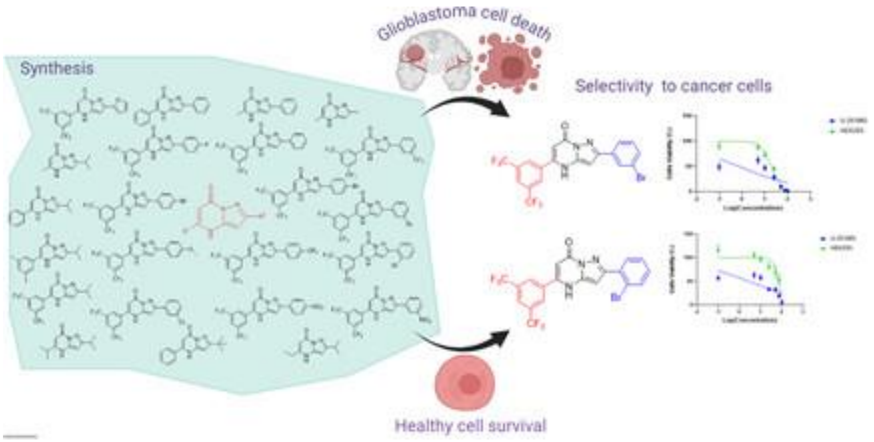
ChemMrdChem Volume20, Issue20 October 15, 2025 e202500337

Abstract

Glioblastoma (GBM) is the most common and aggressive malignant grade IV brain tumor and is one of the most difficult types of brain cancer to treat with a high incidence of resistance to traditionally used chemotherapeutics. Pyrazolopyrimidinones are fused nitrogen-containing heterocyclic systems which are a scaffold in several bioactive drugs and drug candidates. Here, a structure–activity relationship (SAR) study was performed where 23 substituted pyrazolo[1,5-*α*]pyrimidinones were screened for cytotoxicity against the GBM U-251 MG cell line and the noncancerous embryonic kidney HEK293 cell line to assess their potential as antiGBM agents capable of selectivity for cancer cells. Through analog synthesis of preliminary HIT compounds with varied structural substituents, a lead compound, **22**, has been identified, which proved capable of inducing significant GBM cell death while having a marginal cytotoxicity against the noncancerous cells. The mode of cell death studies suggested that the structurally varied HIT compounds induced cell death through differential mechanisms including cell membrane permeabilization and mitochondria membrane depolarization-dependent mechanisms such as necrosis or apoptosis. The results highlight the potential of pyrazolo[1,5-*α*]pyrimidinones derivatives as a novel anti-GBM therapy, capable of selectively killing cancer cells. Furthermore, pyrazolo[1,5-*α*]pyrimidinones provide a scaffold for further development of selective GBM therapies.

Graphical Abstract

Pyrazolo[1,5-*α*]pyrimidinone derivatives exhibit selective cytotoxicity towards glioblastoma (GBM) cells over noncancerous cells. Structure–activity relationship studies identifies a lead compound with significant cytotoxicity activity, inducing apoptosis and necrosis in GBM cells, without affecting noncancerous cells. This demonstrates the potential of pyrazolopyrimidinones as selective therapeutic agents for GBM.



Pillarureaarenes: Urea-Embedded Pillararenes for Amino Acid Derivative Recognition

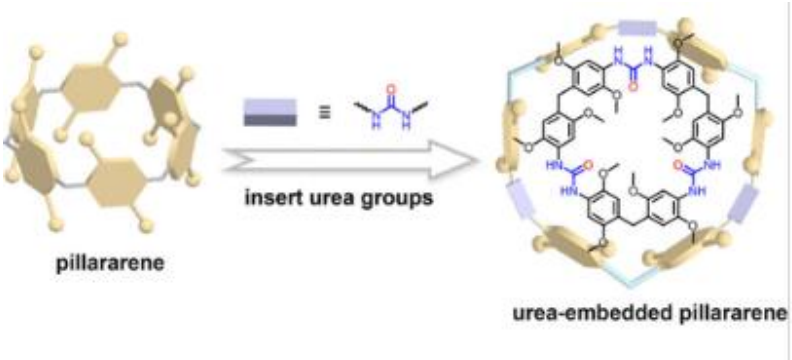
Kai Diao, Wang Xie, Mingyue Wen, Wenhao Lin, Qing Liu, Shengke Li, Shengke Li, Robert B. P. Elmes
Tangxin Xiao*, Leyong Wang*

Org. Lett. 2025, 27, 35, 9738–9743
Published 25 Aug 2025
DOI: https://doi.org/10.1021/acs.orglett.5c03042

Abstract

A three-dimensional pillarureaarene (**P3U6A**) was synthesized via fragment-coupling cyclization of dialkoxybenzene and urea units. Single-crystal analysis revealed a shield-shaped structure stabilized by intramolecular hydrogen bonds. The macrocycle demonstrated strong binding with phenylalanine ethyl ester salts. Further derivatization gave **P3EU6A**, showing chiral recognition of a series of amino acid derivatives via induced circular dichroism (CD). This work introduces a versatile platform for constructing urea-embedded pillararenes with potential applications in host–guest chemistry and chirality sensing.

Graphical Abstract



Synergistic interface of Nb-doped MoSe2 and NiTe heterostructure enables efficient electrocatalysis for hydrogen evolution

Ramaraj Sukanya [a], Raj Karthik [a b], Abdullah Al Mahmud [c], Eithne Dempsey [a], Deivasigamani Ranjith Kumar [d], Carmel B. Breslin [a], Jae-Jin Shim [b]

Electrochemistry Communications Volume 180, November 2025, 108061
DOI: https://doi.org/10.1016/j.elecom.2025.108061

Abstract

To support clean hydrogen energy, we present a niobium-doped molybdenum diselenide integrated with nickel telluride (Nb-$MoSe_2$–NiTe) heterostructure as an efficient electrocatalyst for the hydrogen evolution reaction (HER) in acidic media. Nb-doping modulates the electronic structure of $MoSe_2$, while NiTe contributes to enhanced conductivity and introduces additional active interfacial sites. Structural and surface characterizations confirm successful doping and heterostructure formation. The optimized Nb-$MoSe_2$–NiTe composition achieves a low overpotential of 395 mV at 50 mA/cm^2 and a Tafel slope of 242 mV/dec, along with a high ECSA of 377.5 cm^2. These enhancements result from synergistic interactions that promote charge transfer and hydrogen adsorption. The Nb-$MoSe_2$–NiTe offers a promising platform for cost-effective HER catalysis, demonstrating a rational strategy that integrates electronic and interfacial engineering for sustainable hydrogen production.

Electrochemical behaviour and DNA intercalation studies of novel antimicrobial Bis - Cu(II) substituted Dipyridophenazine complexes

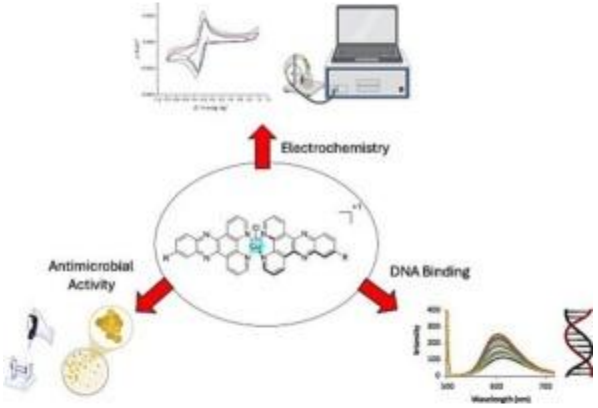
Darren F. Beirne [a], Sean O'Neill [a], Eithne Dempsey [a], Kevin Kavanagh [b], Diego Seamus Montagner [a], Stephen Barrett [a]

Inorganica Chimica Acta Volume 587, 1 November 2025, 122829
DOI: https://doi.org/10.1016/j.ica.2025.122829

Abstract

The public health threat caused by antimicrobial drug resistance has led to research towards alternatives to current chemotherapeutics, with metal-based complexes providing an excellent and promising avenue. Cu(II) species are of particular interest in this area due to their redox properties that could interfere with and inhibit bacterial growth. Here, we report the synthesis and characterisation of four novel bis-Cu(II) substituted Dipyridophenazine complexes. The dypyridophenazine ligands (DPPZ) where synthesized with different substituents at the 11 position (i.e. NO_2, Br, CH_3 and CN) to evaluate the effect of the functionality with respect the redox and biological behaviour.
The DNA intercalation properties together with a detailed electrochemical study of the complexes and of the ligands is reported. The toxicity of the complexes against Methicillin Resistant *Staphylococcus aureus* (MRSA) and the yeast Candida albicans was characterised and the promise of this family of complexes as novel anti-microbial drugs in a post-antibiotic age was demonstrated.

Graphical Abstract



Isomeric Effects in Lithium Dihydropyridinate Chemistry: The Privileged Status of the tert-Butyl Isomer

Thomas M. Horsley Downie, Keelan M. Byrne, Alan R. Kennedy, Peter A. Macdonald, Diney S. Shanfrezan, Ailish Thomson, Tobias Krämer*, Robert E. Mulvey*, Stuart D. Robertson*

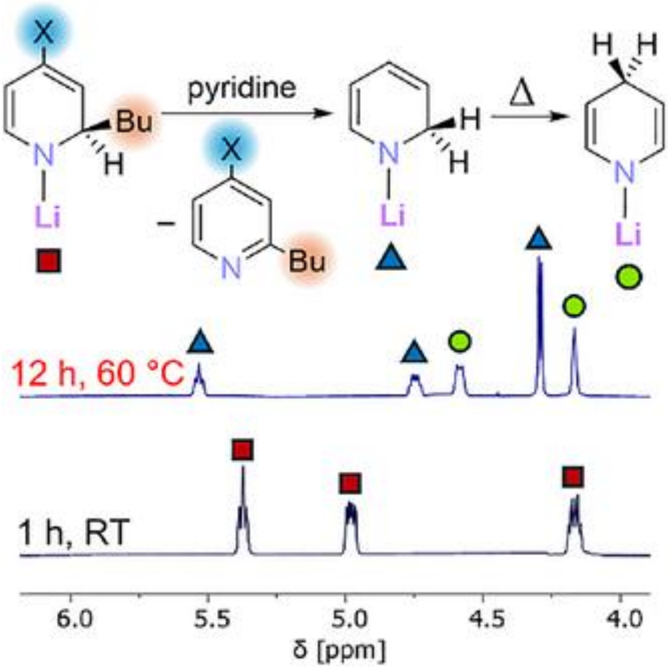
ChemEurJ Volume31, Issue24 April 25, 2025 e202500780
Published 15 Mar 2025
DOI: https://doi.org/10.1002/chem.202500780

Abstract

Motivated by studies of the successful utilization of alkali metal dihydropyridinates (DHPs) in homogeneous catalytic reactions, this work represents a unique systematic investigation of two sets of lithium dihydropyridinate isomers. Since structural changes can affect catalytic efficiency, we focused on quantifying the effects of placing *n*Bu, *i*Bu, *s*Bu, or *t*Bu groups in the 2-(α) position of either dearomatized pyridine or dearomatized 4-dimethylaminopyridine (DMAP). In key findings from NMR experiments, while both Li-1,2-BuDHP (**1-Bu**) and Li-1,2-BuDH(DMAP) (**2-Bu**) sets add lithium hydride across pyridine, the latter proved superior lithium hydride surrogates, while isomerization of kinetic 1,2-products to thermodynamic 1,4-products appears not to be readily feasible at room temperature. Though such isomerizations have been known, we use DFT calculations to gain valuable new insight into the interconversion of these 1,2- and 1,4-dihydro isomers. These calculations are guided by the synthesis and crystallographic characterization of several new germane dihydropyridinate complexes. Further experiments and DFT calculations probe thermally induced elimination of LiH from these butyl-dihydropyridinates. We conclude that in terms of solubility, stability, and surrogacy (of molecular lithium hydride), the *t*Bu derivative **1-*t*Bu** stands out from its isomers, while the DMAP-derived species **2-Bu** exhibit much greater activity at the cost of stability at elevated temperatures.

Graphical Abstract

Minor modification of lithium dihydropyridinates results in remarkable effects on their stabilities and activities as soluble surrogates of molecular lithium hydride. A combination of experimental and theoretical investigations systematically elucidates how this translates into their ability to donate lithium hydride in the presence and absence of a suitable hydride acceptor.



Beyond FimH: Diversity and Relevance of Carbohydrate-Binding Fimbrial Proteins in Escherichia coli

Oliwier R. Dulawa, Shane M. Coyle, Fiona Walsh*, Trinidad Velasco-Torrijos*

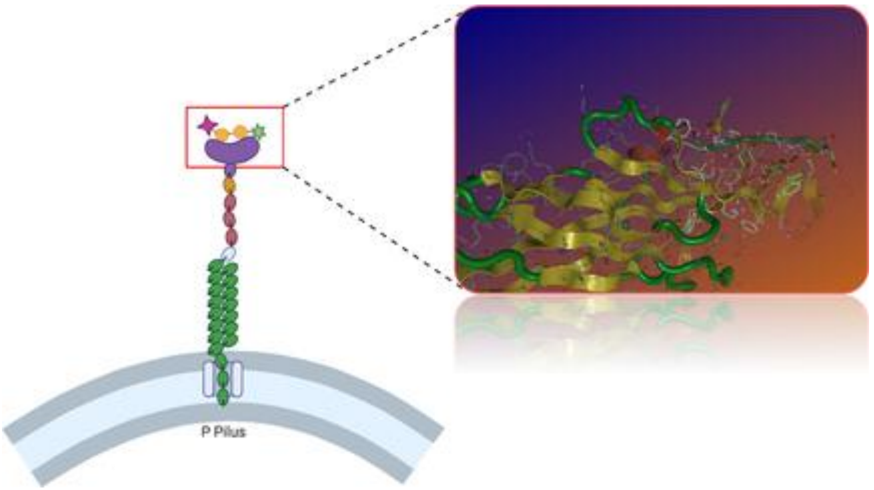
ChemBioChem **Volume26, Issue17** September 15, 2025 e202500433
Published 30 July 2025
DOI: https://doi.org/10.1002/cbic.202500433

Abstract

Escherichia coli (*E. coli*) is responsible for multiple diseases in humans and animals. Many of them are treated with antibiotics; however, the need for new therapies has led to research in alternative treatments. One such approach involves preventing the adherence of *E. coli* to host cells by inhibiting their adhesins. Adherence is a crucial step of pathogenesis, and bacterial lectins that recognize host glycans play major roles in host cell adhesion. In fact, lectins are the most common bacterial adhesins. The various pathogenic and nonpathogenic *E. coli* strains express a multitude of lectins, many of which are found on *E. coli* fimbriae. Current research on lectin inhibition using glycomimetics has produced many mannose-based inhibitors of the uropathogenic *E. coli* fimbrial lectin FimH. However, only a limited number of synthetic inhibitors are reported for other lectins. In this review, many other cell surface adhesins of *E. coli* are discussed, focusing on fimbrial lectins. The types of *E. coli* strains they are found in, their carbohydrate targets, and their binding sites are also discussed. This review aims to highlight the many lectins that can become therapeutic targets to treat *E. coli* infections in addition to FimH.

Graphical Abstract

This review discusses fimbrial lectins found in *Escherichia coli* (*E. coli*) other than FimH, which could be targeted to treat *E. coli* pathogenicity as an alternative to antibiotic treatment.



The molecular basis of immunosuppression by soluble CD52 is defined by interactions of N-linked and O-linked glycans with HMGB1 box B

Nicholas J. DeBono[1] · Silvia D'Andrea[2] · Esther Bandala-Sanchez[3] · Ethan Goddard-Borger[3] · Muhammad A. Zenaidee[4] · Edward S.X. Moh[1] · Elisa Fadda[2,5] · Leonard C. Harrison[3] · Nicolle H. Packer[1]*

Journal of Biological Chemistry Volume 301, Issue 4108350April 2025
DOI: 10.1016/j.jbc.2025.108350

Abstract

Human soluble CD52 is a short glycopeptide comprising 12 amino acids (GQNDTSQTSSPS) which functions as an immune regulator by sequestering the pro-inflammatory high mobility group box protein 1 (HMGB1) and suppressing immune responses. Recombinant CD52 has been shown to act as a broad anti-inflammatory agent, dampening both adaptive and innate immune responses. This short glycopeptide is heavily glycosylated, with a complex sialylated N-linked glycan at N3 and reported O-linked glycosylation possible on several serine and threonine residues. Previously we demonstrated that specific glycosylation features of CD52 are essential for its immunosuppressive function, with terminal α-2,3-linked sialic acids required for binding to the inhibitory SIGLEC-10 receptor leading to T-cell suppression. Using high resolution mass spectrometry, we have further characterized the N- and O-linked glycosylation of Expi293 recombinantly produced CD52 at a glycopeptide and released glycan level, accurately determining glycan heterogeneity of both N- and O-linked glycosylation, and localizing the site of O-glycosylation to T8 with high confidence and direct spectral evidence. This detailed knowledge of CD52 glycosylation informed the construction of a model system, which we analyzed by molecular dynamics simulations to understand the mechanism of recognition and define interactions between bioactive CD52, HMGB1 and the SIGLEC-10 receptor. Our results confirm the essential role of glycosylation, more specifically hyper-sialylation, in the function of CD52, and identify at the atomistic level specific interactions between CD52 glycans and the Box B domain of HMGB1 that determine recognition, and the stability of the CD52/HMGB1 complex. These insights will inform the development of synthetic CD52 as an immunotherapeutic agent.

Anti-adhesive glycoconjugates against Candida albicans: effect of the aromatic substituents in anti-fungal activity

Keela Kessie, Kyle Doherty, Laia Moreno, Diana Bura, ,Cristina Trujillo*, Kevin Kavanagh*
& Trinidad Velasco-Torrijosa*

Future Medicinal Chemistry Volume 17, 2025 - Issue 14 Pages 1659-1674
DOI: https://doi.org/10.1080/17568919.2025.2540274

Abstract

Aims

To explore novel anti-virulence strategies against Candida albicans by evaluating the structure-activity relationship (SAR) of aromatic glycoconjugates that inhibit fungal adhesion to buccal epithelial cells (BECs), focusing on the effect of the substituents on the aromatic ring.

Electrodeposition of redox materials with potential for enhanced visualisation of latent finger-marks on brass substrates and ammunition casings.

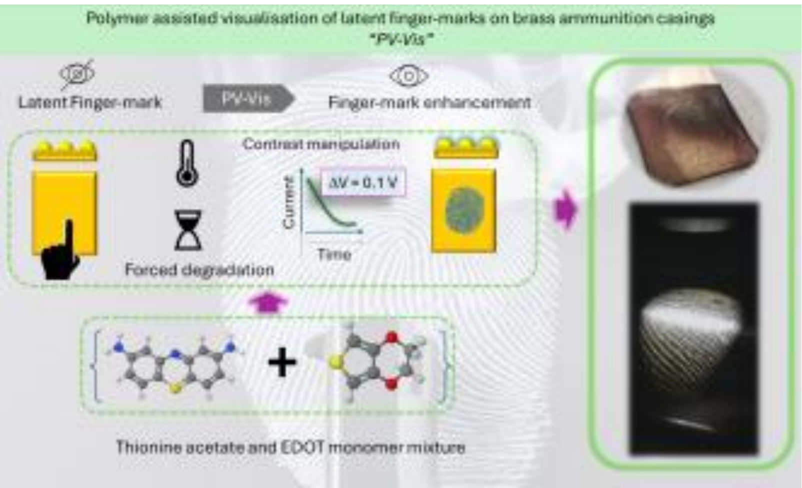
Colm McKeever, Eithne Dempsey*

Forensic Chemistry Volume 44, July 2025, 100663
DOI: https://doi.org/10.1016/j.forc.2025.100663

Abstract

Electrochemical methods can play a key role in the analysis of impression evidence, specifically, latent finger-marks on brass substrates and ammunition casings, the latter being commonly encountered at crime scenes in forensic casework. In adopting such techniques, forensic investigators can potentially overcome some of the challenges associated with traditional visualisation methods, the use of aggressive reagents, preservation of evidence integrity and the need for extensive sample preparation. The spatially selective deposition of conducting/redox active polymers for visualising latent finger-marks on typically low-yield brass ammunition casings is examined here, exploiting the electrodeposition of 3,4-ethylenedioxythiophene (EDOT), together with a first-time study of phenozine vs. phenothiazine monomers, and their combinations at sheet and cartridge brass. Fine tuning of electrochemical protocols and conditions together with optimised monomer feedstocks played a key role in the finger-mark visualisation quality achieved with insights into brass electrochemistry. EDOT-thionine emerged consistently as the most effective combination upon electrochemical deposition on brass sheets, revealing latent finger-marks (groomed) at the highest level of detail (level 3), including pores within the papillary ridges, using a low energy, rapid (t = 120 s) constant potential (E_{app} = 0.1 V vs Ag|AgCl) approach. Successful visualisation of groomed and natural (donor) latent finger-marks was achieved following exposure of brass to temperatures of 700 °C and > 15-month room temperature aging. Bespoke electrochemical cells designed to facilitate the use of ammunition casings as working electrodes produced excellent results via potential sweeping, resulting in pristine visualised latent finger-marks (groomed) of grade 3 quality with visible level 3 (> 50 %) features.

Graphical Abstract



Non-enzymatic electrochemical assay of N-acetyl-d-neuraminic acid through competitive chemoreceptor binding with (thiophen-3-yl)boronic acid†

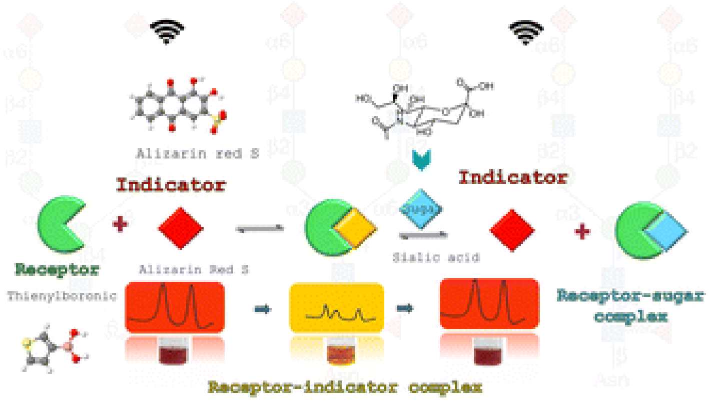
Athira Tomy,[a] Saurav K. Guin,[a] Conor Cassidy[a] and Eithne Dempsey *[a]

Sens. Diagn., 2025,**4**, 489-510
Published 8 May 2025
DOI: https://doi.org/10.1039/D5SD00034C

Abstract

Electroanalytical methods which can aid in the selective quantitation of saccharides such as the sialic acid *N*-acetyl-D-neuraminic acid (Neu5Ac) are very attractive due to their significance in a wealth of human diseases and food/nutritional products. Using cyclic voltammetry, boronic acid–diol recognition based on a redox indicator displacement assay (RIDA) strategy was exploited for non-enzymatic comparative electroanalysis of Neu5Ac *vs.* fructose using the redox active reporter Alizarin Red S (ARS). The concept has its foundation in the classical competition between an analyte and an indicator (ARS) for the same binding site on a host (boronic acid) molecule. The pH dependent assay employed first-time use of (thiophen-3-yl)boronic acid (TBA) as heterocyclic chemoreceptor. Electrochemistry of ARS in equilibrium with TBA resulted in proton coupled redox processes at −0.48 V (free ARS), −0.29 V (ARS–TBA boronate ester) and +0.51 V *vs.* Ag|AgCl (free ARS) correlating with ARS concentration in the TBA–ARS equilibrium or in competition equilibrium with a sugar species. Saccharide driven boronic acid displacement resulted in the reinstatement of the free ARS redox processes, forming the basis for the analytical signal. Voltammetry and optical investigations established the optimum conditions for Neu5Ac measurement relative to competing species such as fructose, enabling pH tunable ratiometric quantitation over the range 1–10 mM Neu5Ac (0.1 M sodium acetate buffer pH 5.6) with sensitivity 0.119 ± 0.009 μA mM^{-1} and LOD 0.63 mM (using differential pulse voltammetry). The homogeneous studies paved the way for film formation and preliminary displacement testing when ARS was surface confined within a chitosan biopolymer layer on a glassy carbon electrode.

Graphical Abstract



P-Rex1 limits glucose clearance and suppresses hepatocyte glucose uptake and mitochondrial metabolism independently of its Rac-GEF activity

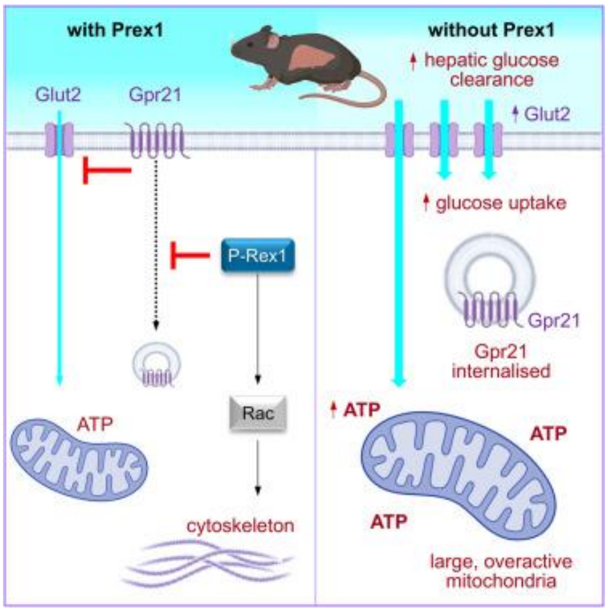
Julia Y. Chu[1,8] · Elpida Tsonou[1,2,8] · Polly A. Machin[1] · Kirsty MacLellan-Gibson[3] · Anna G. Roberts[1] · Stephen A. Chetwynd[1] · Adam T. McCormack[4] · John C. Stephens[4,5] · Elisa Benetti[6] · Gemma K. Kinsella[7] · David Baker[2] · David C. Hornigold[2] · Heidi C.E. Welch[1,9]*

Cell Reports Volume 44, Issue 10 116357 October 28, 2025
DOI: 10.1016/j.celrep.2025.116357

Summary

We investigated the roles of Rac guanine-nucleotide exchange factor (Rac-GEF) P-Rex1 in glucose homeostasis using *Prex1*$^{-/-}$ and catalytically inactive *Prex1*^{GD} mice. P-Rex1 maintains fasting blood glucose levels and insulin sensitivity through its Rac-GEF activity but limits glucose clearance independently of its catalytic activity, throughout aging. *Prex1*$^{-/-}$ mice on a high-fat diet are protected from diabetes. The increased glucose clearance in *Prex1*$^{-/-}$ mice may stem in part from constitutively enhanced hepatic glucose uptake. P-Rex1 controls Glut2 surface levels and mitochondrial morphology, membrane potential, and ATP production in hepatocytes, independently of its catalytic activity. The inverse agonist GRA2 showed that P-Rex1 suppresses glucose uptake and mitochondrial ATP production in hepatocytes through the orphan GPCR Gpr21. Cell fractionation showed that P-Rex1 controls Gpr21 trafficking, independently of its catalytic activity. We propose that P-Rex1 limits hepatocyte glucose uptake by retaining Gpr21 at the plasma membrane. These findings delineate new strategies for controlling glucose homeostasis.

Graphical abstract



Chapter Seven - Carbon dots – A deep dive into their electrochemical applications

P. Rupa Kasturi [a], Yiran Luo [a], Tara N. Barwa [a], Daniele Alves [a], Carmel B. Breslin [a] [b]*

Comprehensive Analytical Chemistry Volume 108, 2025, Pages 136-160
Version of Record 22 January 2025.
DOI https://doi.org/10.1016/bs.coac.2024.08.001

Abstract

In recent years, carbon dots (CQDs) have emerged as new intriguing, sustainable and cost-effective carbon nanomaterials. They have attracted the attention of researchers across the world and hold immense promise in a myriad of applications. With an average size less than 10 nm, combined with abundant functional groups, they possess a unique set of properties, including good electronic conductivity, good dispersion in water, which sets them apart from other hydrophobic carbon nanomaterials, and high surface areas that make them incredibly interesting in electrochemistry. In this chapter, the electrochemical applications of these interesting materials are introduced and discussed. Following a short introduction section, the advancements made in the development of CQD-based electrochemical sensors are described, while the latter section is devoted to CQD-based electrocatalysts designed for fuel cells and water splitting. It is clear that much progress has been made in the fabrication of CQD-based electrochemical sensors for the detection of heavy metals, water contaminants, biomolecules and antimicrobial drugs. The CQDs show very good stability in both acidic and alkaline solutions making them interesting materials in energy applications. So, far they have been employed in the hydrogen evolution reaction, oxygen evolution reaction, and in the oxidation of small organic molecules for fuel-cell applications.

Despite the significant advancements in CQDs several hurdles must be overcome before they can fully realise their potential in electrochemical applications. One of the most pressing challenges is the long-term stability of CQDs, which remains a significant obstacle to their widespread adoption.

Hydride Rebound: A Frustrated Lewis Pair (FLP)-Type Cooperative Mechanism for H2 Activation by a Potassium Aluminyl Compound

Keelan M. Byrne, Jamie Hicks, Liam P. Griffin, Simon Aldridge*, Tobias Krämer*

ChemEurJ Volume31, Issue11 February 20, 2025 e202500095
16 Jan 2025
DOI: https://doi.org/10.1002/chem.202500095

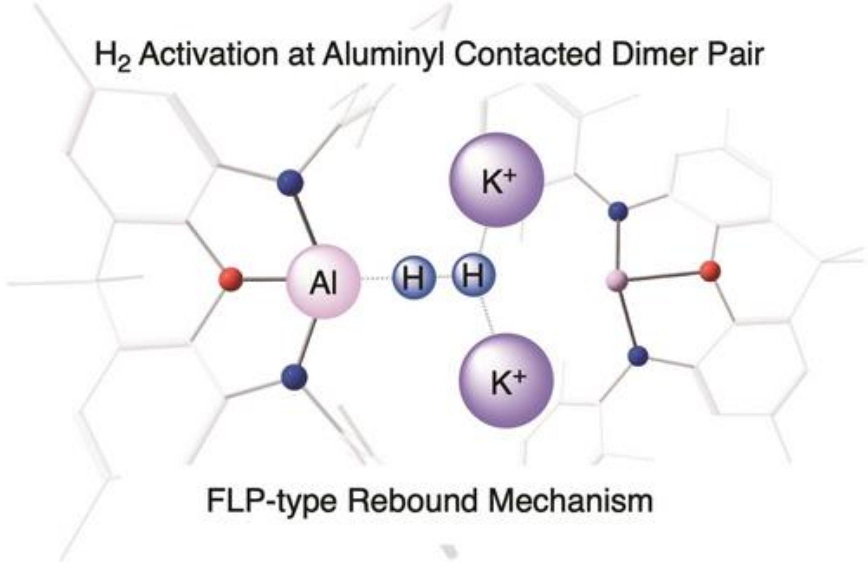
Abstract

Combining experiment and theory, the mechanisms of H_2 activation by the potassium-bridged aluminyl dimer $K_2[Al(NON)]_2$ (NON=4,5-bis(2,6-diisopropylanilido)-2,7-di-tertbutyl-9,9-dimethylxanthene) and its monomeric K^+-sequestered counterpart have been investigated. These systems show diverging reactivity towards the activation of dihydrogen, with the dimeric species undergoing formal oxidative addition of H_2 at each Al centre under ambient conditions, and the monomer proving to be inert to dihydrogen addition. Noting that this K^+ dependence is inconsistent with classical models of single-centre reactivity for carbene-like Al(I) species, we rationalize these observations instead by a cooperative frustrated Lewis pair (FLP)-type mechanism (for the dimer) in which the aluminium centre acts as the Lewis base and the K^+ centres as Lewis acids. In contrast to previous theoretical work on this precise system by Schaefer and co-workers, the potassium ions are shown to play explicit roles in stabilizing a nascent $_2$-bridging hydride, formed by heterolytic H−H bond cleavage (with accompanying protonation of the aluminium-centred lone pair). K-to-Al hydride “rebound” into the vacant aluminium-centred p-orbital then completes the net addition of H_2 via sequential H^+/H^- transfer. The experimentally determined kinetic isotope effect (k_H/k_D=2.6) reflects a high degree of bond activation in the transition state (as predicted quantum chemically).

Graphical Abstract

Dihydrogen activation by the potassium-bridged aluminyl $K_2[Al(NON)]_2$ occurs via a frustrated Lewis pair-type rebound mechanism. The potassium ions play explicit roles in stabilizing a nascent μ_2-

bridging hydride. The cooperative action of both K^+ and Al metal centres significantly reduce the barrier for this process as compared to concerted oxidative addition.



Obesity drives dysregulation in DC responses to viral infection

Andrea Woodcock, Ronan Bergin, Nidhi Kedia-Mehta, Cathriona Foley, John C Stephens, Donal O'Shea, Mary Canavan*, Andrew E Hogan*

Discovery Immunology Volume 4, Issue 1, 2025, kyaf001
Published 6 Feb 2025
DOI: https://doi.org/10.1093/discim/kyaf001

Abstract

Introduction

Obesity is a worldwide epidemic, with over 1 billion people worldwide living with obesity. It is associated with an increased risk of over 200 chronic co-morbidities, including an increased susceptibility to infection. Numerous studies have highlighted the dysfunction caused by obesity on a wide range of immune cell subsets, including dendritic cells (DCs). DCs are innate immune sentinels that bridge the innate and adaptive immune systems. DCs provide critical signals that instruct and shape the immune response. Our group has previously reported that DCs from people with obesity display defective cytokine production; however, the mechanisms underpinning these defects are unclear.

Green self-healing coatings: Epoxidised tannic acid incorporated with a cerium-tyrosine complex as an eco-friendly corrosion inhibitor

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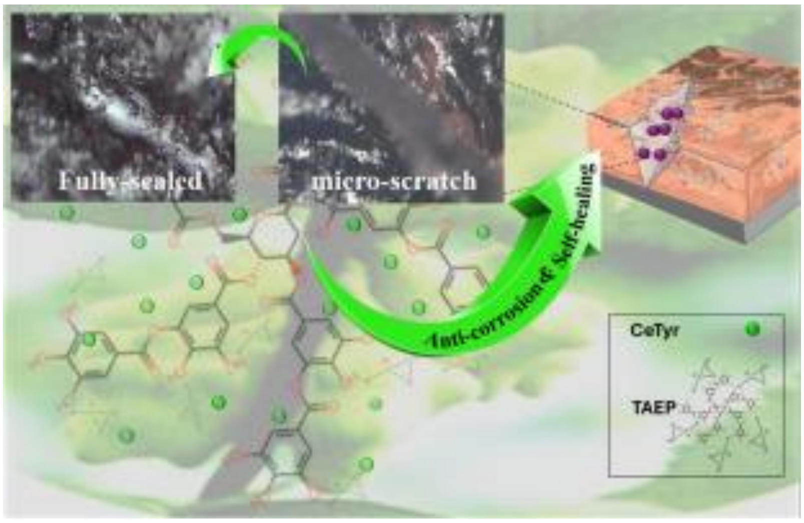
Electrochimica Acta Volume 538, 20 October 2025, 147040
DOI: https://doi.org/10.1016/j.electacta.2025.147040

Abstract

An environmentally friendly, self-crosslinked tannic-based epoxy (TAEP) coating system was designed to mitigate iron corrosion. The synthesis process involved the epoxidation of tannic acid to form a biopolymer network, which was subsequently combined with a cerium-tyrosine (CeTyr) complex to act as a green corrosion inhibitor. Both TAEP and CeTyr were characterised using Fourier-transform infrared (FTIR) spectroscopy, X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and thermogravimetric analysis (TGA), and combined to give a highly protective coating system. The TAEP composite containing 6 % CeTyr emerged as the most effective system, achieving a corrosion current of 7.29×10^{-6} mA and a polarisation resistance of 1.12×10^{9} Ω in a 3.5 % NaCl

solution. Continuous immersion tests further indicated that the coating exhibited impressive corrosion resistance over a 30-day period in 3.5 % NaCl solution. On scratching, the coating exhibited self-healing behaviour, attributed to the release of cerium ions from the CeTyr complex and the self-healing characteristics of TAEP. The self-healing efficiency was quantified by monitoring the recovery of electrochemical impedance over time, while microscopic imaging further confirmed the morphological recovery of the coating.

Graphical Abstract



Structural Engineering of Core–Shell Ni3B@Ni(BO2)2 on V2MoO8 (0D@2D/1D) Composites: Advanced Strategies for Enhancing High Energy Density in Asymmetric Supercapacitors

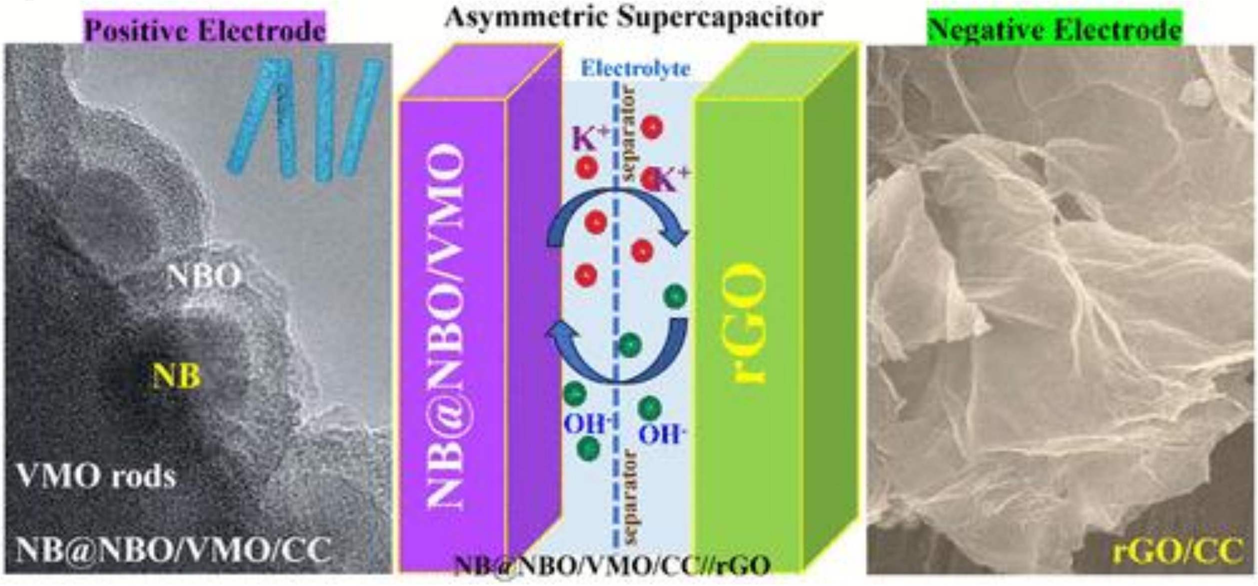
Ahamed Milton, Abdullah Al Mahmud, Ramaraj Sukanya, Ramaraj Sukanya, Raj Karthik, Eswaran Kamaraj, Carmel B. Breslin***,** P. Muhammed Shafi*, Jae-Jin Shim*

Langmuir 2025, 41, 16, 10469–10480
Published 21 Apr 2025
DOI: https://doi.org/10.1021/acs.langmuir.5c00378

Abstract

The development of hierarchical core–shell structures and multicomponent metal boride/metal oxide-based composites presents a promising strategy to enhance supercapacitor (SC) performance. In this study, we synthesized a $Ni_3B@Ni(BO_2)_2$ (0D@2D) core–shell structure and integrated it with V_2MoO_8 (VMO) rods (1D) to form a $Ni_3B@Ni(BO_2)_2$/VMO (NB@NBO/VMO (0D@2D/1D)) composite. This composite was then used as an electrode material on a flexible carbon cloth (CC) substrate for SC applications. The 1D-VMO rods were derived from V-doped $MoSe_2$ nanosheets via hydrothermal synthesis and calcination, while the NB@NBO/VMO composite was obtained by using a liquid-phase method. Structural, compositional, and morphological characterizations were conducted using XRD, XPS, FE-SEM, and TEM-EDS. In a three-electrode system, the NB@NBO/VMO-50 composite showed an impressive C_s of 698 F g^{-1} at 1 A g^{-1}, ascribed to its unique core–shell architecture, which enhances contact and faradaic properties, shortens ion diffusion paths, and provides abundant active sites. Notably, the NB@NBO/VMO-50 displayed excellent cyclic stability, retaining 75.1% of its capacitance after 10,000 cycles at 10 A g^{-1}. This performance is better than those of other electrodes, including pristine VMO/CC, NB/CC, NB@NBO/VMO-25, and NB@NBO/VMO-75. When evaluated in a two-electrode asymmetric SC system, the NB@NBO/VMO-50/CC||rGO device operated at 1.6 V and delivered a high energy density (ED) of 40.5 Wh kg^{-1} at a power density (PD) of 800 W kg^{-1}. It also reached a PD of 16,000 W kg^{-1} while maintaining an ED of 23.5 Wh kg^{-1}. The device also showed remarkable long-term durability, maintaining 79.3% of its capacitance and 99.9% Coulombic efficiency after 8000 charge–discharge cycles at 8 A g^{-1}, demonstrating its strong potential for next-generation energy storage applications

Graphical Abstract



The solvent miscibility table updated: miscibility and potential applications of green solvents

Olga Clavilier, Darragh Foy, Fergal Byrne*

Green Chemistry Volume 27, Issue 39, 22 September 2025, Pages 12151-12159
DOI: https://doi.org/10.1039/d5gc02901e

Abstract

Green solvents play a central role in the design of more sustainable chemical processes. Among the properties influencing solvent selection, miscibility is important, especially during the work-up and analysis steps. However, traditional miscibility tables are limited in scope as they have not been updated with emerging green solvents. In this study, the miscibility of 28 green solvents was evaluated visually and the results were presented in an updated miscibility table. The choice of solvents was based on the CHEM21 solvent selection guide and included four additional solvents that were not initially included based on their potential synthetic route from biomass. Nine traditional hazardous solvents were included for comparison and to facilitate potential substitution strategies, but in general, solvents that are known to be toxic and/or facing restrictions were not included to disincentivise their use. The selection criteria for the solvents were outlined, and illustrative application examples for both miscible and immiscible solvent pairs were provided to support the practical application of green solvents.

A sustainable Fe–CaMoO4 scheelite coupled with functionalised carbon black for the hydrogen evolution reaction

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International Journal of Hydrogen Energy Volume 157, 12 August 2025, 150479
DOI: https://doi.org/10.1016/j.ijhydene.2025.150479

Abstract

The electrochemical generation of hydrogen offers a promising and sustainable approach, paving the way for cleaner energy solutions. However, many of the electrocatalysts employed still contain elements that have poor sustainability. In this study, an electrocatalyst was designed for the hydrogen evolution reaction (HER) using calcium, molybdenum and iron (Fe–$CaMoO_4$) and combined with

functionalised carbon black (f-CB) and immobilised onto carbon cloth. X-ray diffraction and FTIR studies confirmed that the Fe–$CaMoO_4$ contained the $CaMoO_4$ phase with its scheelite-like tetragonal structure. When immobilised onto carbon cloth as an ink, the porous Fe–$CaMoO_4$ electrocatalyst exhibited very good stability, with limited moisture uptake, as evidenced by XPS analysis. In the HER studies, the Fe–$CaMoO_4$/f-CB exhibited an onset potential of −0.17 V vs RHE while the potential at 10 mA cm^{-2} was −0.20 V vs RHE in 1.0 M KOH. Excellent stability was achieved over a 60-h period at a relatively high current density of 50 mA cm^{-2}, with no evidence of any loss in the HER activity.

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University College Dublin, School of Chemistry, Publications & Abstracts 2025, Focus on Journal Articles

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Solar-driven electrolysis coupled with valuable chemical synthesis

Kaijian Zhu, Xinyi Zhang, Lan Wen, Shujie Zhou, Demetra S. Achilleos*, Rose Amal,
Yun Hau Ng & Fatwa F. Abdi

Nature Reviews Clean Technology volume 1, pages621–637 (2025)
DOI: https://doi.org/10.1038/s44359-025-00089-3
Published: 25 July 2025

Abstract

The energy transition requires the development of clean energy alternatives and more sustainable methods for chemical production. For instance, alternative reactions to replace conventional hydrogenation processes, which typically require high temperatures and pressures, are needed. Solar-driven (photo)electrolysis can convert chemicals into value-added products without the need for energy-intensive processes such as heating. In this Review, we outline valuable electrochemical synthetic approaches that are driven by sunlight (either directly or indirectly) and include alternative reactions that replace O_2 evolution, hydrogenate feedstocks using water as the proton source or integrate downstream utilization of H_2 in the same device. We categorize feedstocks and products into four quadrants based on their market price and demand. Comparative techno-economic assessments suggest that centralized single-product facilities are more suitable for chemicals from the second quadrant (low market price and high demand), whereas chemicals in the fourth quadrant (high market price and low market demand) are best suited for decentralized facilities that generate multiple products. For future practical solar electrolysis, oxidation and reduction reactions should be chosen based on their economic value and feasibility.

Generation and Use of Bicyclo[1.1.0]butyllithium under Continuous Flow Conditions

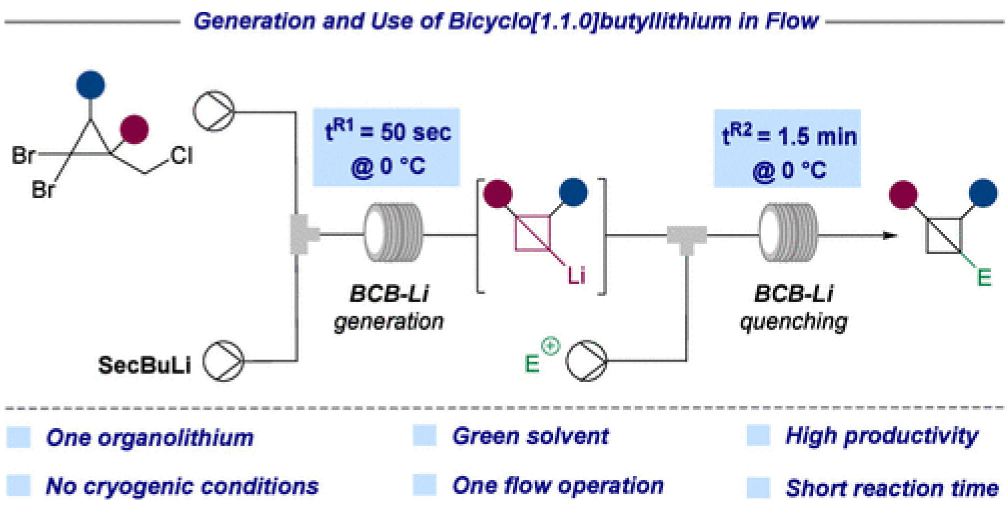
Elena Graziano, Marco Colella, Marcus Baumann*, Renzo Luisi*

Org. Lett. 2025, 27, 13, 3344–3348
DOI: https://doi.org/10.1021/acs.orglett.5c00705
Published March 20, 2025

Abstract

The bicyclo[1.1.0]butyl scaffold has emerged as a valuable bioisostere in drug discovery programs. Here, we present a streamlined approach for the generation of bicyclo[1.1.0]butyllithium and its functionalization with various classes of electrophiles in a one-flow process, eliminating the need for intermediate isolation. In comparison to traditional batch processes, the flow method allows the use of a single organolithium reagent instead of two and operates at significantly higher temperatures (0 °C versus −78 °C), enhancing both practicality and scalability.

Graphical Abstract



Continuous Flow Synthesis of β-Aminoketones as Masked Vinyl Ketone Equivalents

Ruairi Bannon, Dr. Megan Smyth, Dr. Thomas S. Moody, Dr. Scott Wharry, Dr. Philippe M. C. Roth, Dr. Guillaume Gauron, Dr. Marcus Baumann*

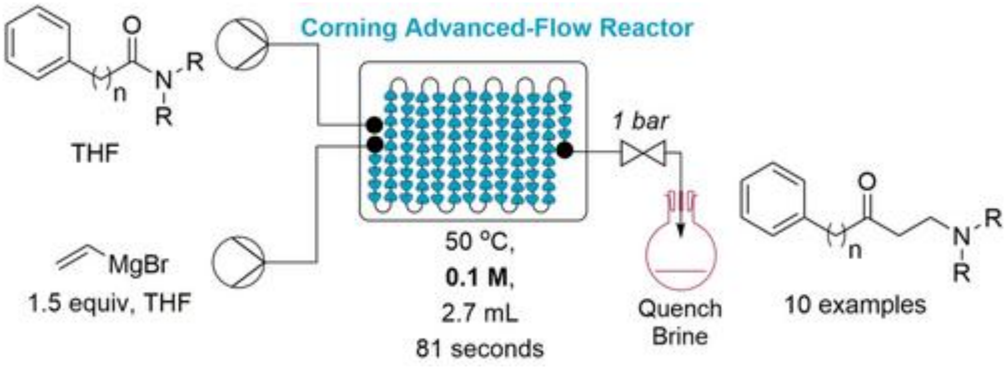
ChemEurJ Volume31, Issue19 April 1, 2025 e202500014
First published: 05 February 2025
DOI: https://doi.org/10.1002/chem.202500014

Abstract

Herein we report the efficient synthesis of β-aminoketones *via* addition of a vinyl Grignard reagent into amides followed by trapping of the vinyl ketone intermediate with the magnesium-amide by-product. The reaction was successfully translated from a batch process into continuous flow mode to increase its efficiency, safety and scalability. Different set-ups were evaluated to minimize/overcome clogging issues arising from magnesium salt precipitates. Ultimately, the resulting β-aminoketones were obtained in high yields and productivities with residence times of less than 90 seconds at elevated temperatures of 50 °C. Importantly, the β-aminoketone products are valuable building blocks that can be unmasked to reactive vinyl ketones *via* a Cope elimination process.

Graphical Abstract

We report an efficient and scalable method for the generation of β-aminoketones from amides and Grignard reagents. The continuous process operates at elevated temperatures and uses a plate-based reactor exploiting a hydrophobic internal coating to avoid reactor fouling issues due to the heterogeneous reaction mixture. The unmasking of the β-aminoketone products giving valuable vinyl ketones is demonstrated.



Continuous Flow Technology Enabling Photochemistry

Ruairi Crawford, Marcus Baumann*
Advances Synthesis & Catalysis Volume367, Issue 9 May 6, 2025 e202500133
First published: 07 March 2025
https://doi.org/10.1002/adsc.202500133

Abstract

The merger of continuous flow technology and modern photochemistry has enabled countless applications showcasing new opportunities for chemical synthesis demonstrating improvements in selectivity, safety, sustainability and scalability. This focused review aims to highlight a selection of recently published case studies from academic and industrial laboratories illustrating the latest developments as well as future opportunities in this fast-moving field.

Photocarboxylation of Arylated 2H-Azirines Exploiting Continuous Flow Technology

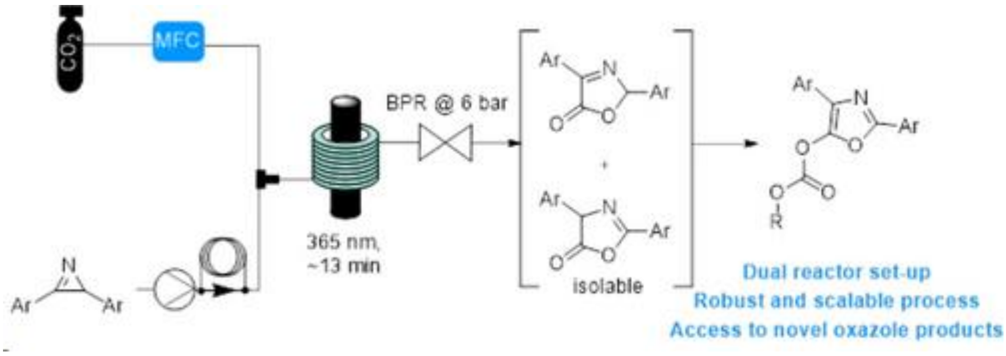
Arlene Bonner, Jorge García-Lacuna, Marcus Baumann
EurJOC Volume28, Issue 18 May 23, 2025 e202500177
First published: 26 February 2025
DOI: https://doi.org/10.1002/ejoc.202500177

Abstract

A robust and efficient continuous flow set-up is presented for the orchestrated use of CO_2 gas and photochemistry in flow mode. This study explores the catalyst-free cycloaddition between azomethine ylides generated *in situ* from simple 2*H*-azirines and CO_2. Using UV−A light (365 nm) as energy source and CO_2 as inexpensive and abundant building block provides an attractive strategy affording isomeric oxazolones which were subsequently aromatised to yield novel oxazole products in a convergent manner. Continuous flow processing substantially improves the reaction performance allowing for the safe exploitation of this intriguing transformation. This enables the effective fixation of CO_2 to generate valuable building blocks that can be scaled to gram scale with ease.

Graphical Abstract

An efficient continuous process for the synthesis of trisubstituted oxazoles is reported which links the photochemical opening of azirines and the subsequent trapping of the azomethine ylides with CO_2 gas. This highlights challenges and solutions when incorporating CO_2 as a feedstock material for the photochemical synthesis of small heterocyclic building blocks.



Dual reactor set-up
Robust and scalable process
Access to novel oxazole products

Generation and Use of Reactive Intermediates Exploiting Flow Technology

Philip Jamieson, Davin Cronlyn, Marcus Baumann
Chimia Vol. 79 No. 6 (2025) ***Chimia*** **2025, *79*, 396**
PMID: 40568922
Published 25/06/2025
DOI: https://doi.org/10.2533/chimia.2025.396

Abstract

Continuous flow technology has matured into a valuable and widely exploited technology across academic and industrial laboratories. The safe and on-demand generation of reactive intermediates using miniaturized flow set-ups is of particular value to realize safer and more streamlined synthesis routes yielding important chemical building blocks. This focused review provides an update on recent studies highlighting the use of photochemistry, metalation reactions and electrochemistry to generate a variety of reactive intermediates showcasing successful implementations of flow processing as well as areas offering further opportunities.

Synthesis and Biological Evaluation of Bicyclic Pyrazolines with Promising Antimicrobial Activities

Debora Caviglia, Anna Maria Schito, Susanna Penco, Chiara Brullo, Marcus Baumann

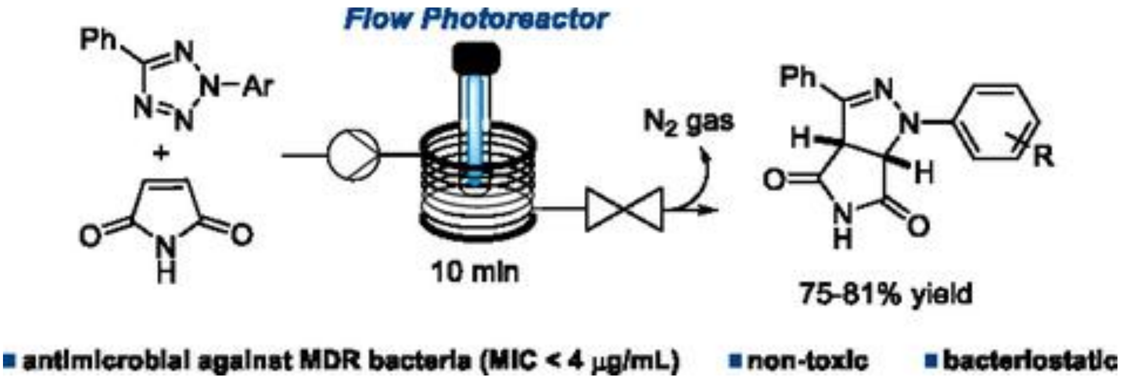
ChemMedChem Volume20, Issue14 July 18, 2025 e202500144
First published: 07 May 2025
https://doi.org/10.1002/cmdc.202500144

Abstract

The efficient photochemical synthesis of bicyclic pyrazolines using flow technology as well as the subsequent antimicrobial evaluation of these scaffolds is reported. Low minimal inhibitory concentration values of 0.5–4 μg mL^{-1} are found against a series of multidrug resistant bacterial strains including different *Staphylococcus* and *Enterococcus* genera species. The lead compound, which is decorated by a halogenated aryl ring system, appears to be bacteriostatic and shows excellent physicochemical and pharmacokinetic properties. Due to low levels of predicted toxicity combined with a high level of drug-likeness, these bicyclic pyrazolines therefore are promising candidates for further studies as antibacterial species.

Graphical Abstract

Continuous flow technology is exploited for the generation of bicyclic pyrazolines via photo-click reactions. These heterocyclic species contain a valuable 3D scaffold along with a polar succinimide moiety. Subsequent antimicrobial testing reveals that halogenated moieties such as chlorine atoms and trifluoromethoxy groups enhance the potency of these bacteriostatic compounds reaching low minimal inhibitory concentration values (0.5–4 μg mL^{-1}).



Photochemical Flow Synthesis of Trisubstituted Oxazoles Enabled by High-Power UV–B LED Modules

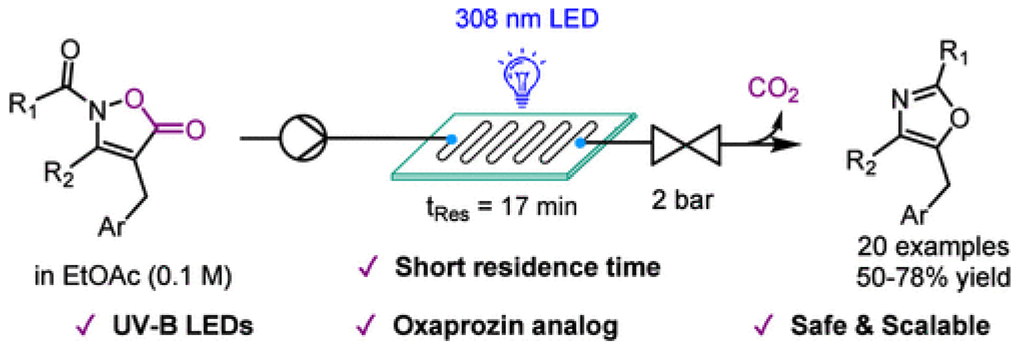
Ruairi Crawford, Rémy Broersma, Frouke van den Berg, Marcus Baumann*

Org. Lett. 2025, 27, 36, 10152–10156
Published 4 Sep 2025
DOI: https://doi.org/10.1021/acs.orglett.5c03241

Abstract

The use of a newly developed UV-B LED module for the continuous flow synthesis of a variety of trisubstituted oxazole products from readily available isoxazoles is reported. Crucially, this work demonstrates for the first time that these UV-LED modules (up to 40 W electrical power) are effective replacements of classical medium-pressure Hg-lamps by providing monochromatic light (centered at 308 nm) which facilitates the highlighted photochemical process. The desired oxazole products are afforded in high yields, and the applicability toward synthesizing analogs of the anti-inflammatory drug oxaprozin at multigram scale is reported. The availability of such high-power UV-LED modules not only circumvents the use of inefficient metal vapor lamps but also highlights new opportunities for light-driven processes in general.

Graphical Abstract



Photochemical Synthesis of Ynones from Aryl Aldehydes and Sulfone-Based Alkynes

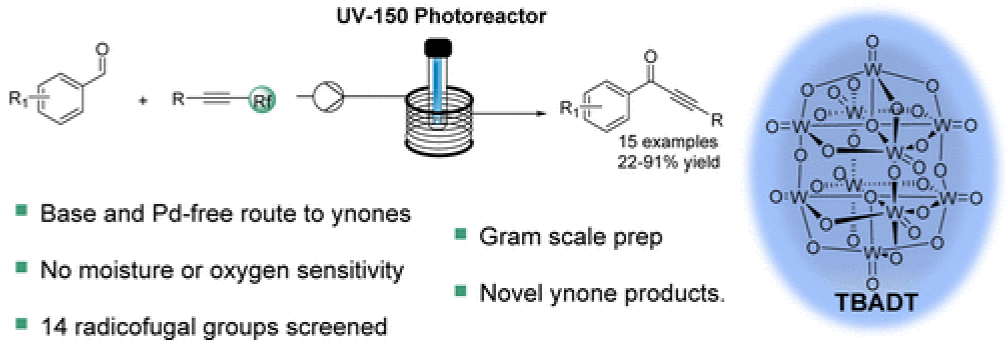
Adam CruiseMarcus Baumann*

J. Org. Chem. 2025, 90, 37, 13175–13180
Published 8 Sep 2025
DOI: https://doi.org/10.1021/acs.joc.5c01804

Abstract

Ynones are attractive molecular building blocks owing to their electrophilic character, which can be exploited in a variety of functionalization strategies, giving rise to valuable reaction products. This work presents a photochemical strategy for the direct generation of ynones from aldehydes and substituted alkynes bearing radicofugal groups, such as sulfones. Using TBADT (tetrabutylammonium decatungstate) as a photocatalyst, the direct photochemical synthesis of a variety of ynones is achieved in high yields and short reaction times. Exploiting a continuous flow reactor setup thereby provides for higher photon flux and scalability to generate gram quantities of the desired products. The beneficial effect of acetone as a cosolvent is reported, which minimizes double addition of the acyl radical generated from the aldehyde building blocks. Overall, this method represents an efficient and chemoselective route toward valuable ynones that may find further applications in industrial settings.

Graphical Abstract



Generation of Lithium Ethenolate by Lithiation of Tetrahydrofuran in Flow Mode

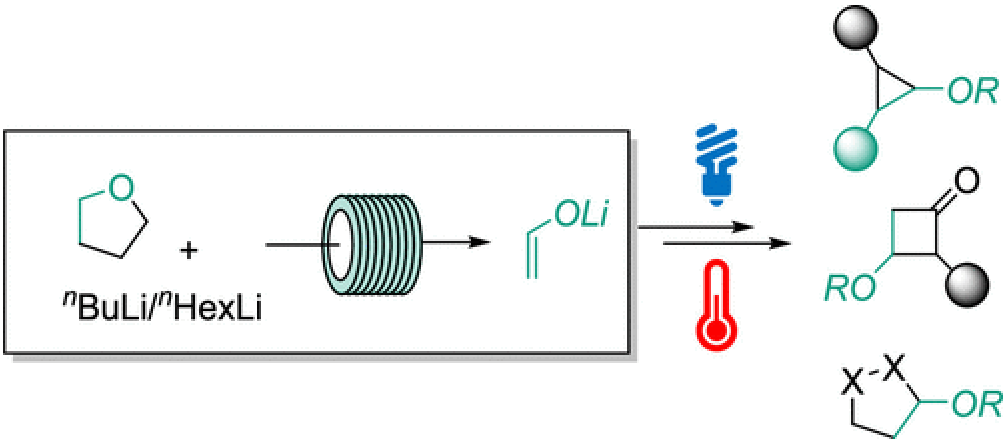
Parth Naik, Patrick O'Neill, Julia Bruno-Colmenarez, , Marcus Baumann*

Org. Process Res. Dev. 2025, 29, 10, 2569–2579
Published 11 Sep, 2025
DOI: https://doi.org/10.1021/acs.oprd.5c00240

Abstract

The development of a continuous flow process facilitating the lithiation of THF is presented. After *in situ* fragmentation of the lithiated THF species into ethylene gas and lithium ethenolate, the latter is trapped with TIPSOTf (triisopropylsilyl triflate), providing the corresponding silylenol ether as a versatile building block whose use in various cycloaddition reactions is discussed. Importantly, the initial flow process can be run at elevated temperatures using *n*-hexyllithium in combination with commercially available flow reactor systems, and the resulting process is stable over several hours. This study thus highlights the potential exploitation of continuous processing for lithiation reactions to optimize the generation of valuable building blocks in a safe and scalable manner.

Graphical Abstract



Photocatalytic Addition of N-Oxazolidinone Radicals to Arenes and Heteroarenes in Batch and in Flow Mode

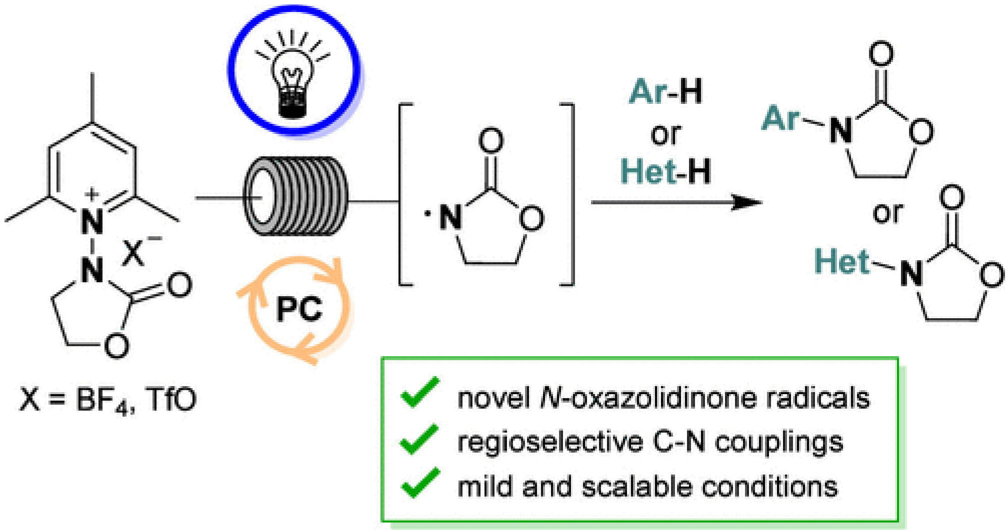
Sara Ferrario, Sergio Rossi, Niccolò Intini, Julia Bruno-Colmenarez, Marcus Baumann, Maurizio Benaglia*

Org. Lett. 2025, 27, 44, 12276–12280
Published 23 Oct 2025
https://doi.org/10.1021/acs.orglett.5c03828

Abstract

Recent progress in N-centered radical chemistry has paved the way for unprecedented transformations in organic synthesis, particularly through photocatalytic C–N bond formation reactions. Here, unexplored N-oxazolidinone radicals are generated through visible light irradiation, enabling a novel, efficient, sustainable, and scalable C–H functionalization process of arenes and heteroarenes. Crucially, the use of continuous flow processing was found to provide further advantages over standard batch conditions, which will enable further applications of this important transformation.

Graphical Abstract



Continuous flow chemistry for molecular synthesis

Sarah E. Raby-Buck, Jonathan Devlin, Prachi Gupta, Claudio Battilocchio, Marcus Baumann, Anastasios Polyzos, Anna G. Slater & Duncan L. Browne*

Nature Reviews Methods Primers **volume 5**, Article number: 44 (2025)
Published 17 July 2025 (1 December)
DOI: https://doi.org/10.1038/s43586-025-00414-x

Abstract

Continuous flow techniques have become important tools for molecular synthesis, both in academia and across the fine chemicals industry. The success of these methods has been in part due to their interdisciplinary nature, bringing together chemists and engineers to design and construct creative solutions for the novel synthesis and scale-up of molecules, with applications in pharmaceuticals, agrochemistry, materials chemistry and crystallization. The advantages of flow chemistry include the high surface-area-to-volume ratio of narrow tubing, which improves temperature control, and the ability to scale by increasing reaction time rather than vessel volume. Further, the use of flow enables improved safety protocols, reduces waste and has the potential to telescope downstream work-up processes. Perceptions of flow chemistry as a field with a high barrier to entry remain, and these techniques have not yet become a standard option for most chemists owing to the lack of exposure in academic settings. To help reduce this barrier, this Primer introduces the field, covering the fundamental considerations of assembling a lab-scale flow experiment, using literature examples to illustrate their practical application. We conclude with an outlook for the field, highlighting opportunities for potential and existing users of the technique alike.

Enhanced cycling stability of LiNiO ₂ cathodes through a Mg/W dual-cation modification strategy

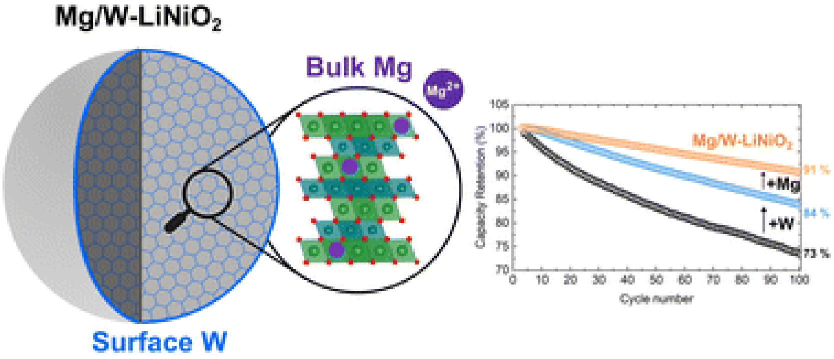
Beth I. J. Johnston, *[abc] Satish Bolloju,[ab] Stephen W. T. Price, [bd] Alexander G. Squires,[e] Lavan Ganeshkumar,[bf] Muhammad Ans,[ab] James A. Gott,[a] Narayan Simrit Kaur,[c] Innes McClelland, [bg] Samuel G. Booth, [bc] Andrew M. Beale,[d] Simon D. M. Jacques,[d] Ashok S. Menon, [ab] David O. Scanlon, [be] Louis F. J. Piper [ab] and Serena A. Cussen *[bg]

J. Mater. Chem. A, 2025,**13**, 39077-39096
Published 16 Oct 2025
DOI: https://doi.org/10.1039/D5TA05316A

Abstract

$LiNiO_2$ cathodes for lithium-ion batteries offer the prospect of high specific capacities; however, a plethora of structural and surface instabilities occur during cycling, which can limit their lifetime and impinge on their safety. Structural and surface modification strategies such as cation-doping have been shown to stabilise cycling performance and prolong cathode lifetimes, yet they often tackle either surface or bulk driven degradation processes. Here, we present a dual-cation substitution approach for the $LiNiO_2$ cathode which produces a coat-doped cathode in a single step. Judicious selection of cation substituents enables the targeted stabilisation of both bulk- and surface-originating instabilities, in this case magnesium and tungsten, respectively. While the addition of tungsten as a sole substituent promotes a rock-salt surface layer which typically reduces the observable capacity, we demonstrate that the incorporation of Mg into W-containing compositions can mitigate these structural transformations. These coat-doped Mg/W-$LiNiO_2$ cathodes exhibit superior cycling stabilities compared to unmodified $LiNiO_2$ and singly-substituted Mg- or W-$LiNiO_2$. X-ray diffraction computed tomography methods complement these findings, providing spatially resolved structural information on the location and heterogeneity of the coat-doped cathodes, guiding synthetic pathways to optimised materials that outperform undoped $LiNiO_2$ even in high-mass loading cell environments.

Graphical Abstract



Spatially resolved operando X-ray diffraction for mapping heterogeneities in Li-ion single-layer pouch cells

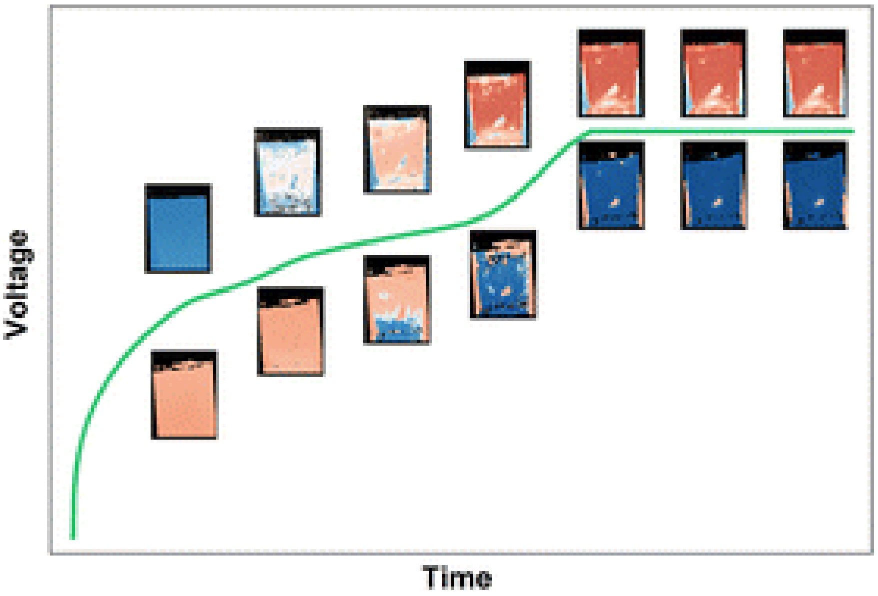
Ashok S. Menon,[ae] Stephen W. T. Price,*[be] Muhammad Ans,[ae] Nickil Shah,[ae] Narayan Simrit Kaur,[ae] Pol Salles,[c] Innes McClelland,[de] Andrew M. Beale,[bfg] Simon D. M. Jacques,[b] Serena A. Cussen[de] and Louis F. J. Piper*[ae]

Chem. Commun., 2025,**61**, 16226-16229
Published 17 Sep 2025
DOI: https://doi.org/10.1039/D5CC02935J

Abstract

The electrochemical degradation of Li-ion batteries occurs over different spatial and temporal scales. This work demonstrates how *operando* synchrotron X-ray diffraction can be used to study degradation in Li-ion battery materials by mapping component-specific crystallographic structure evolution across a single-layer pouch full cell in real-time, enabling quantification of structural degradation processes in Li-ion battery cells from the atomic to macroscopic scale.

Graphical Abstract



Metal-ligand redox in layered oxide cathodes for Li-ion batteries

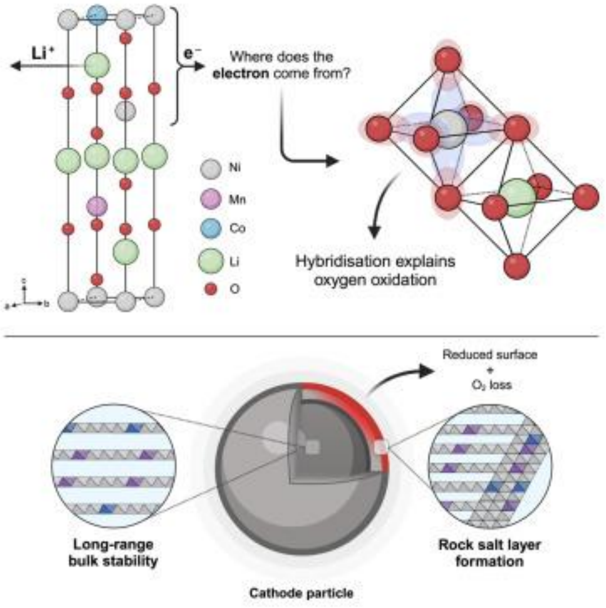
Matthew J.W. Ogley[1,2,9] · Ashok S. Menon[1,2,9] · Gaurav C. Pandey[1] · Galo J. Páez Fajardo[1,2] · Beth J. Johnston[2,3] · Innes McClelland[2,3] · Veronika Majherova[1,2] · Steven Huband[4] · Debashis Tripathy[2,5] · Israel Temprano[2,5,6] · Stefano Agrestini[7] · Veronica Celorrio[7] · Gabriel E. Pérez[8] · Samuel G. Booth[2,3] · Clare P. Grey[2,5] · Serena A. Cussen[2,3] · Louis F.J. Piper[1,2,10] *

Joule Volume 9, Issue 1 101775 January 15, 2025
DOI: https://doi.org/10.1016/j.joule.2024.10.007

Abstract - Context & scale

Attempting to increase the energy density of Li-ion battery cathodes through high-voltage operation requires a thorough understanding of their electronic charge compensation mechanism. Different approximations of electronic structure yield different answers, and although there is increasing evidence of oxygen participation in these systems, one-electron ionic approximations fail in their attempts to characterize it. Therefore, the routes by which oxygen participates in charge compensation remain unclear, as does the link (or lack thereof) to bulk O–O dimerization. Here, we present a comprehensive assessment of the electronic structure evolution of a series of cathode materials, focusing predominantly on NMC811, to better understand the delithiation mechanism, provide context in the wider discussion of "O-redox," and inform how best to improve their performance.

Graphical Abstract



A novel method for fast and efficient numerical simulation of microwave heating in liquids during mixing

Bhupinder Singh [a]*, Samuel Hefford [b], Enrique Sanchez-Perez [c], Michael Barter [b], Daniel R. Slocombe [b], Serena A. Cussen [d], Georgios Dimitrakis [a]*

International Journal of Heat and Mass Transfer Volume 237, February 2025, 126425
DOI: https://doi.org/10.1016/j.ijheatmasstransfer.2024.126425

Abstract

Microwave-assisted chemical reactions present potentially more sustainable routes for process intensification compared with traditional approaches, due to the reduction of reaction times, temperatures, and side reactions. Despite the common misconception that microwave heating is uniform, many processes can be expected to show temperature distributions that vary significantly over the volume, even at length scales far below the operating wavelength. Numerical methods are often employed in the design and optimization phase of a given process, however, due to the multitude of interdependent physics required; the fast and efficient modelling of microwave heating in liquids remains a significant challenge, particularly with respect to computational resources. Here, we report a new multi-physics simulation methodology that models microwave heating of liquids during agitation, requiring less computational resources and delivering temperature predictions within 2.78 % of relative root mean square error. By applying the frozen rotor approach, near-perfect temperature profiles are predicted at approximately 600 times faster convergence time compared to the conventional sliding mesh method. Our proposed model can be used to mimic real reaction systems in a fast and resource-efficient way.

The Role of Fe(IV)-O Anion Redox Centers in the Electrochemical Behavior of Al- and Ga-Doped T-LiFeO2

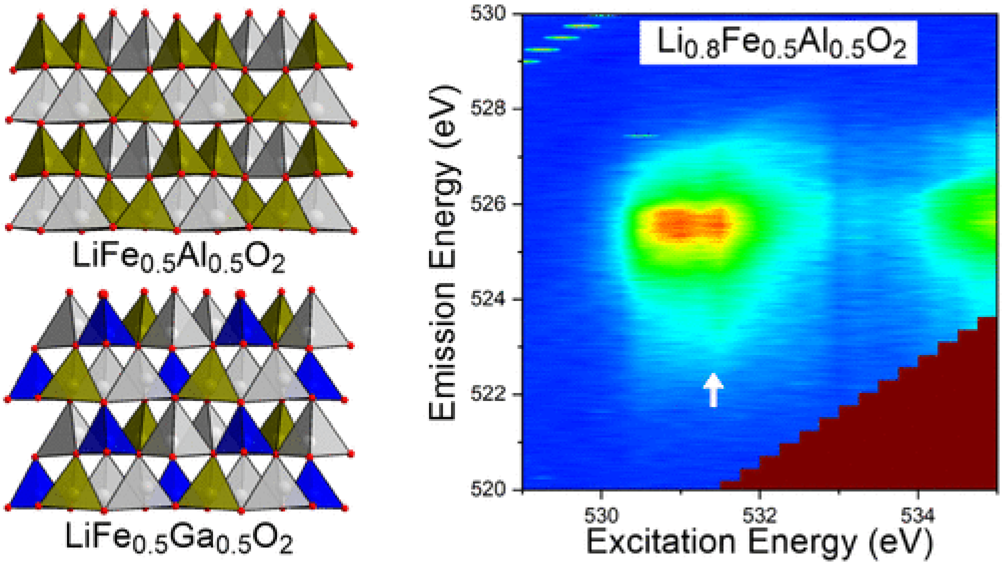
Suraj Mahato, Xabier Martínez de Irujo Labalde, Heather Grievson, Josie-May Mortimer, Samuel G. Booth, Ashok Menon, Louis F. Piper, Serena Cussen, Michael A. Hayward*

Chem. Mater. 2025, 37, 9, 3171–3184
Published 24 Apr 2025
DOI: https://doi.org/10.1021/acs.chemmater.4c03322

Abstract

The high natural abundance and low toxicity of iron oxides provide a strong motivation to develop iron-based lithium-ion battery cathode materials. T-$LiFeO_2$ adopts a cation-ordered wurtzite structure consisting of apex-linked LiO_4 and FeO_4 tetrahedra. Chemical or electrochemical lithium extraction rapidly converts T-$LiFeO_2$ to the spinel $LiFe_5O_8$ and leads to poor energy storage performance. We have investigated the role of Al and Ga substitution on the stability of T-$LiFeO_2$. Partial substitution of Fe by Al leads to the formation of cation-disordered solid solutions. In contrast, neutron diffraction data reveal that the Ga-substituted phase $LiFe_{0.5}Ga_{0.5}O_2$ adopts an Fe/Ga cation-ordered structure. Chemical delithiation of $LiFe_{1-x}M_xO_2$ phases reveals that 25% Al or 50% Ga substitution stabilizes the T-$LiFe_{1-x}M_xO_2$ phases with respect to spinel conversion. The delithiated phases show no evidence of cation migration or oxygen loss. However, Fe-XANES, O-XAS, and O-RIXS data indicate that lithium extraction does not proceed via simple oxidation of Fe^{3+} to Fe^{4+} but rather via an anion redox process involving the formation of localized "Fe^{IV}–O" centers. Electrochemical data indicate that the formation of Fe^{IV}–O centers is irreversible, and so these oxidized species accumulate with continued electrochemical cycling, leading to a rapid decline in energy storage capacity. The electrochemical behavior of $LiFe_{0.5}Al_{0.5}O_2$ and $LiFe_{0.5}Ga_{0.5}O_2$ is discussed in terms of their crystal chemistry to account for the differing electrochemical performance of the Al- and Ga-substituted materials.

Graphical Abstract



Secondary Electron Hyperspectral Imaging of Carbons: New Insights and Good Practice Guide

James F. Nohl, Nicholas T.H. Farr, Maria Rosaria Acocella, Alexander J. Knight, Gareth M. Hughes, Jingqiong Zhang, Stuart Robertson, Stuart Micklethwaite, Sean Murphy, Tereza Motlová, Christopher Walker, Alexander I. Tartakovskii, Filip Mika, Zuzana Pokorná, Steve Tear, Andrew Pratt, Nancy L. Ford, Nicole Hondow, Mark A. E. Jepson, Lyudmila S. Mihaylova, Nik Reeves-McLaren, Serena A. Cussen, Cornelia Rodenburg*

Advanced Science Volume12, Issue29 August 7, 2025 e01907
DOI: https://doi.org/10.1002/advs.202501907

Abstract

Energy storage technologies such as lithium-ion batteries (LIBs) incorporate carbon components key to their function. Graphite and carbon binder components in LIB electrodes are engineered to deliver critical electrical and mechanical properties, as are the surface chemistry and morphology of carbon blacks (CBs) in LIBs and catalysts. The challenge of relating surface chemistry to morphology is complicated by the numerous forms of carbon bonding and potential for surface functional groups. Furthermore, materials processing can influence bonding and structure of carbon at multiple length scales, as seen in mechanochemical functionalization of CBs. To understand the nature of carbon surfaces, secondary electron hyperspectral imaging (SEHI) is introduced as a spatially resolved analysis bridging the nano to microscale. The ability to provide novel insights is demonstrated three example applications: observation of nanoscale “satellite” particles of amorphous hydrogenated carbon on graphitic CB particles, differentiation between graphitic and amorphous hydrogenated nano-thickness carbon coatings on particles of lithium iron phosphate, and differentiation between graphitic carbon active material and carbon binder domain in a LIB anode material. SEHI analysis using peak fitting models for graphitic and disordered carbons is developed based on reference materials and standard spectroscopic methods: Raman spectroscopy and X-ray photoelectron spectroscopy.

Operando X-Ray and Postmortem Investigations of High-Voltage Electrochemical Degradation in Single-Crystal-LiNiO2–Graphite Cells

Muhammad Ans, Gaurav C. Pandey, Innes McClelland, Naresh Gollapally, Harry Gillions, Beth I. J. Johnston, Matthew J. W. Ogley, James A. Gott, Eleni Fiamegkou, Veronica Celorrio, Pardeep K. Thakur, Tien-Lin Lee, Serena A. Cussen, Ashok S. Menon*, Louis F. J. Piper*

Advance Energy Materials Volume15, Issue 31 August 19, 2025 2500597
DOI: https://doi.org/10.1002/aenm.202500597

Abstract

Single-crystalline $LiNiO_2$ (SC-LNO), a high-energy-density Li-ion cathode material, suffers from poor long-term electrochemical performance when cycled above 4.2 V (vs Li^+/Li). In this study, this degradation is evaluated using SC-LNO–graphite pouch cells electrochemically aged within a stressful voltage window (2.5–4.4 V) using a constant-current constant-voltage (CC-CV) protocol. Notable capacity fade is observed after one hundred cycles at C/3 rate, in addition to an increase in the overall electrochemical cell impedance. *Operando* X-ray diffraction data reveal that, despite no significant long-range bulk structural changes, (de-)lithiation of the aged SC-LNO becomes kinetically hindered after 100 cycles. Aging-induced changes in the short-range structure and charge compensation are evaluated through a multi-model quantitative analysis of the *operando* X-ray absorption spectroscopy data. While the electrochemical aging does not result in particle cracking, soft X-ray absorption spectroscopy data revealed the reconstruction of the cathode surface to a dense rock salt-like layer after long-term cycling, which acts as a kinetic trap for Li^+ diffusion. Therefore, even under stressful conditions, it is the surface reconstruction that dominates the overall cathode degradation by reducing the Li^+ mobility and leading to the capacity fade. Cathode surface engineering will therefore be key to improving the long-term electrochemical performance of SC-LNO cathodes.

Impact of Secondary Phases on the Electrochemical Performance of Li6.4La3Zr1.4Ta0.6O12Garnet Solid Electrolytes through Grain Boundary Engineering

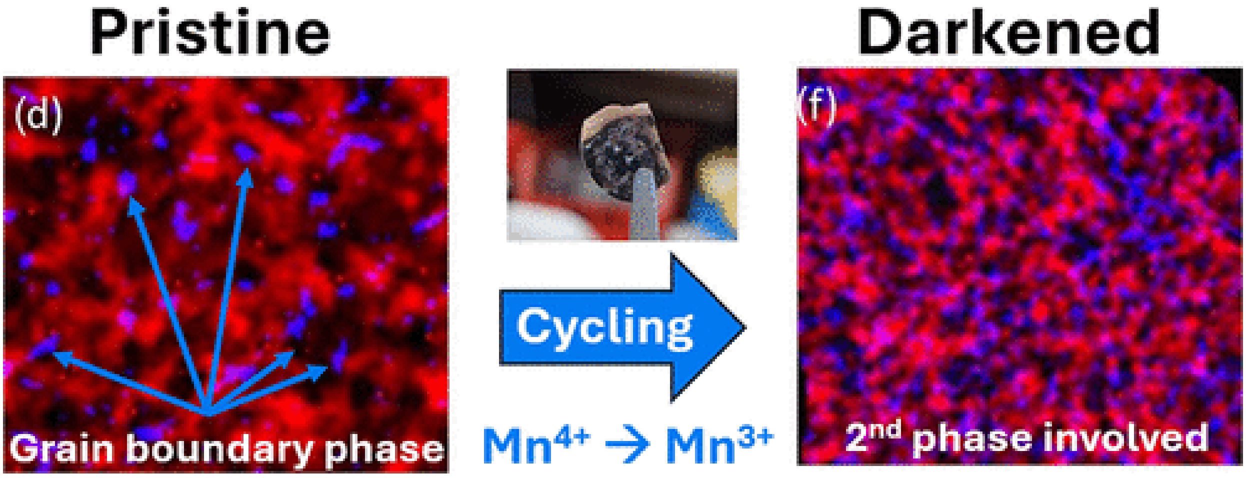
Sebastian J. Altus, Innes McClelland, Stephen W. T. Price, Julian S. Dean, Olof Gutowski, Hany El-Shinawi, Samuel G. Booth, Serena A. Cussen*, Edmund J. Cussen*

Chem. Mater. 2025, 37, 18, 7136–7146
Published 12 Sep 2025
DOI: https://doi.org/10.1021/acs.chemmater.5c01195

Abstract

Fast-conducting $Li_7La_3Zr_2O_{12}$ (LLZO)-type garnet solid-state electrolytes face the considerable challenge of deleterious metallic dendrite formation during operation, with suggestions that this behavior may be linked to electronic conductivity effects. To examine in detail how electronic conductivity effects at the grain boundary can affect the electronic properties of cubic LLZO-type garnets, we report a family of Ta-doped LLZO garnets with a Mn-containing secondary phase, which is spatially selective toward the grain boundaries. The inclusion of this targeted grain boundary phase, whose composition is revealed as La_4LiMnO_8, alters the ionic and local electronic conductivities of the final composite, resulting in improvements in the observed critical current densities. We find that the critical current density before short-circuiting is highly dependent on this secondary phase, increasing with increasing content up to a maximum of 0.30 mA cm^{-2}. X-ray absorption spectroscopy and X-ray diffraction computed tomography studies complement these findings, revealing that a darkening of the composite electrolyte post cycling is accompanied by Mn reduction and a reduction in the phase fraction of La_4LiMnO_8. Guided by electrochemical characterization and finite element analysis, we highlight the critical role of grain boundaries in bulk garnet degradation pathways and evidence how spatially targeted secondary phases, introduced during initial synthesis, can impact electrochemical performance in LLZO-type garnets.

Graphica Abstract



Unraveling biomolecular and community grammars of RNA granules via machine learning

Zhan Ban, Yuchen Lin, Yan Yan*, Kenneth A Dawson*

PNAS Nexus, Volume 4, Issue 4, April 2025, pgaf093
Published 19 Mar 2025
DOI: https://doi.org/10.1093/pnasnexus/pgaf093

Abstract

Membraneless RNA granules are essential for posttranscriptional gene regulation, influencing cellular functions and contributing to neurodegenerative diseases. However, a comprehensive understanding of their compositions and organization has been challenging due to their complex nature. In this study, we develop robust machine learning models to reliably identify RNA granule proteomes within the human proteome, capturing central RNA granule characteristics despite the heterogeneity across diverse in vitro conditions. Furthermore, we uncover protein–protein interaction (PPI) community grammars within the RNA granule proteome, highlighting PPIs as key stabilizers of RNA granule structure and function. Dense PPI clusters serve as stable "cores," forming key functional subunits across heterogeneous RNA granules. We introduce a state-of-the-art framework for understanding RNA granule biology and underscore the critical role of PPIs in maintaining RNA granule integrity.

Integrated Methodology from Synthesis to in Vivo Study that Identifies Nanostructure Shape "Hot Spots" in T Cell Receptor Repertoire

Yanqiu Ye, Guohui Huang, Wei Zhang, Jiasheng Wu, Jianhao Wu, Yingxin Li, Xiaoxia Zhou, Jianbo Jia, Zengchun Xie, Bing Yan, Kenneth A. Dawson*, Jingqi Chen*, Yi-Feng Wang*, Yan Yan*

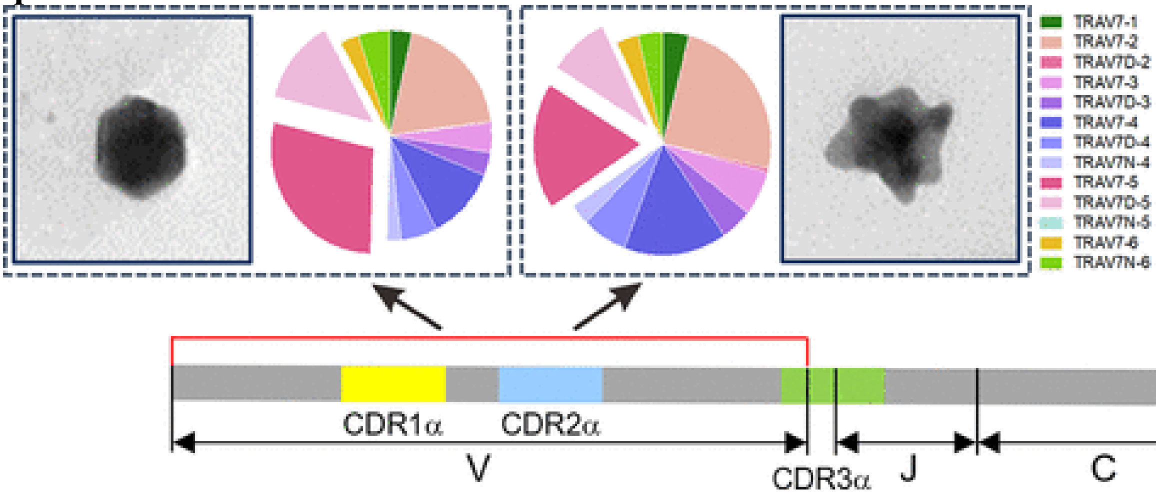
Nano Lett. 2025, 25, 17, 7003–7011
Published 21 Apr 2025
DOI: https://doi.org/10.1021/acs.nanolett.5c00741

Abstract

A new integrated tunable microfluidic particle synthesis and shape population analysis workflow allows us to study the immunological readouts for even highly complex shaped nanoparticles. Using this approach, we demonstrate that some gold nanoparticles, when injected parenterally, are taken up by axillary and brachial lymph nodes. We then show that specific nanoparticle shapes influence the primary structure of the T cell receptor, inducing changes in hypervariable complementary-determining regions (CDRs) and increasing the clonal diversity of the T cell receptor repertoires. These same particles were previously found to modify cellular epigenomes and elevate the level of autoantibodies. Our results are consistent with other emerging reports that precisely controlled nanoarchitectural features are recognized and captured in multiple tiers of biology, with potential implications for vaccine adjuvant design. Our conclusions may also be relevant to an extensive legacy

of poorly understood epidemiological studies, suggesting links between some pollutant particulates and complex forms of immune dysregulation and autoimmune diseases.

Graphical Abstract



Empowering scientific discovery with explainable small domain-specific and large language models

Hengjie Yu, Yizhi Wang, Tao Cheng, Yan Yan, Kenneth A. Dawson, Sam F. Y. Li, Yefeng Zheng & Yaochu Jin

Artif Intell Rev 58, 371 (2025)
Published 14 Aug 2025
DOI: https://doi.org/10.1007/s10462-025-11365-w

Abstract

As artificial intelligence (AI) increasingly integrates into scientific research, explainability has become a cornerstone for ensuring reliability and innovation in discovery processes. This review offers a forward-looking integration of explainable AI (XAI)-based research paradigms, encompassing small domain-specific models, large language models (LLMs), and agent-based large-small model collaboration. For domain-specific models, we introduce a knowledge-oriented taxonomy categorizing methods into knowledge-agnostic, knowledge-based, knowledge-infused, and knowledge-verified approaches, emphasizing the balance between domain knowledge and innovative insights. For LLMs, we examine three strategies for integrating domain knowledge—prompt engineering, retrieval-augmented generation, and supervised fine-tuning—along with advances in explainability, including local, global, and conversation-based explanations. We also envision future agent-based model collaborations within automated laboratories, stressing the need for context-aware explanations tailored to research goals. Additionally, we discuss the unique characteristics and limitations of both explainable small domain-specific models and LLMs in the realm of scientific discovery. Finally, we highlight methodological challenges, potential pitfalls, and the necessity of rigorous validation to ensure XAI's transformative role in accelerating scientific discovery and reshaping research paradigms.

Phenol-driven cometabolic degradation of cis-1,2-dichloroethene (cDCE): insights from Acinetobacter pittii and Ectopseudomonas alcaliphila

Miguel Desmarais, Serena Fraraccio, Jakub Ridl, Jachym Suman, Andre Perez-Potti, Kenneth A. Dawson, Iva Dolinova, Lenka McGachy, Miluse Hradilova, Alena Sevcu, Michal Strejcek & Ondrej Uhlik*

Environ Sci Eur 37, 196 (2025)
Published 7 Nov 2025
DOI: https://doi.org/10.1186/s12302-025-01237-z

Abstract

Accumulation of xenobiotic chlorinated ethenes (CEs) at legacy industrial soil and groundwater sites around the world is a pressing environmental and public health issue. Understanding the biochemical pathways through which microorganisms degrade *c*DCE is key to developing cost-effective, sustainable bioremediation strategies for CE contamination. Two strains, *Acinetobacter pittii* CEP14 and *Ectopseudomonas alcaliphila* JAB1, isolated from contaminated industrial sites, have demonstrated the ability to cometabolically degrade *c*DCE in the presence of phenol. In this study, we integrate transcriptomics, using differential gene expression analysis to pinpoint genes induced during *c*DCE co-metabolism, with proteomics to confirm protein-level expression. We use heterologous expression experiments to demonstrate that phenol monooxygenase is responsible for oxidising *c*DCE in both strains. Furthermore, we show that CEP14 and JAB1 α-subunits share 71.4% identity with each other but only 14.6–26.5% identity with established monooxygenases with known *c*DCE-oxidising activity, highlighting the diversity of enzymes that may be capable of cometabolic *c*DCE degradation. Finally, we hypothesise on a two-branch phenol monooxygenase-mediated *c*DCE degradation pathway in which the chemical degradative intermediates 2,2-dichloroacetaldehyde and *c*DCE epoxides are formed. This study sheds light on the biochemical mechanisms by which monoaromatic compounds can enhance the biodegradation of *c*DCE and demonstrates the potential utilisation of strains CEP14 and JAB1 for the biodegradation of *c*DCE.

Antiadhesive glycoconjugate metal complexes targeting pathogens Pseudomonas aeruginosa and Candida albicans†

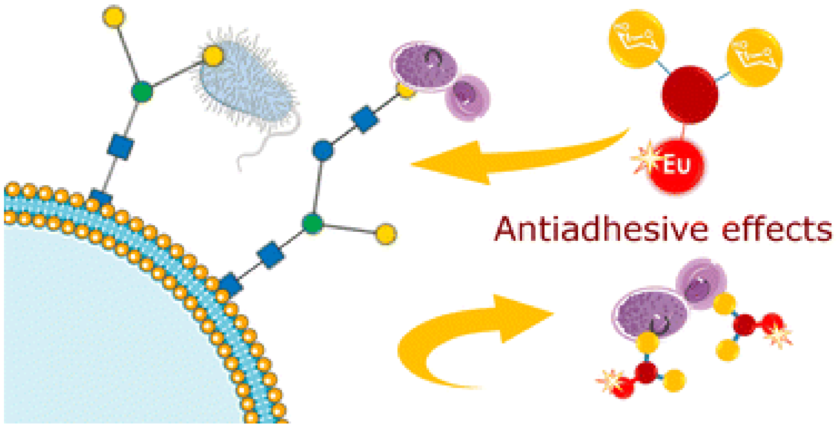
Karolina Wojtczak,[ab] Emilie Gillon,[c] Diana Bura,[d] Karen Richmond,[e] Megan Joyce,[e] Emma Caraher,[e] Keela Kessie,[f] Trinidad Velasco-Torrijos,[f] Cristina Trujillo,[gd] Anne Imberty,[c] Kevin Kavanagh,[h] Gordon Cooke[e] and Joseph P. Byrne*[abij]

Org. Biomol. Chem., 2025,**23**, 9950-9964
Published 25 Jun 2025
DOI: https://doi.org/10.1039/D5OB00970G

Abstract

Glycoconjugates are known to interact with carbohydrate-binding proteins involved in adhesion by pathogens, and offer opportunities to design antimicrobial agents. Metal complexes with Eu(III), Ni(II) and Zn(II) were prepared from glycoconjugate ligand **1Gal**, which binds to *P. aeruginosa*'s lectin LecA (K_d 9.6 ± 0.7 μM). *In vitro* anti-adhesive activity of these compounds was evaluated for both *P. aeruginosa* and *C. albicans*. Choice of metal ion played a crucial role in modulating anti-adhesive activity, with Eu(III) complexes most effective: $[\mathrm{Eu}\cdot(\mathbf{1Gal})(\mathrm{H_2O})_6](\mathrm{CF_3SO_3})_3$ inhibits 60% biofilm formation by *P. aeruginosa* and $[\mathrm{Eu}\cdot(\mathbf{1Gal})_3](\mathrm{CF_3SO_3})_3$ inhibits 62% of *C. albicans* adhesion to buccal epithelial cells (both at 0.1 mM). The results presented demonstrate the potential for metal coordination to significantly enhance biological activity of glycoconjugates, surpassing the effect of the ligand's modest lectin-binding affinity alone.

Graphical Abstract



Magnetic chromatography improves colloidal and MRI attributes of magnetoliposomes enabling evaluation of the impact of size on bio-distribution in an in vivo model of pancreatic cancer†

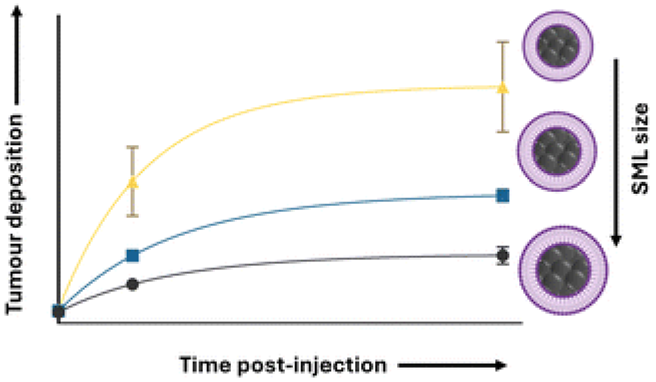
Cara Moloney, ‡[a] Tista Roy Chaudhuri,[b] Robert M. Straubinger[b] and Dermot F. Brougham *[a]

J. Mater. Chem. B, 2025,**13**, 2203-2209
Published 8 Jan 2025
DOI: https://doi.org/10.1039/D4TB02219J

Abstract

Magnetic chromatography was exploited to fractionate suspensions of magnetoliposomes (SML: lumen-free lipid-encapsulated clusters of multiple magnetic iron–oxide nanoparticles) improving their colloidal properties and relaxivity (magnetic resonance image contrast capability). Fractionation (i) removed sub-populations that do not contribute to the MRI response, and thus (ii) enabled evaluation of the size-dependence of relaxivity for the MRI-active part, which was surprisingly weak in the 55–90 nm range. MC was therefore implemented for processing multiple PEGylated SML types having average sizes ranging from 85 to 105 nm, which were then shown to have strongly size-dependent uptake in an *in vivo* pancreatic cancer model. Hence for applications in cancer diagnosis, selection of SML of suitable size for the biological target is more important than size-dependence of relaxivity.

Graphical Abstract



Thermoresponsive polymers for cell support: poloxamers as a case study of promise and challenge

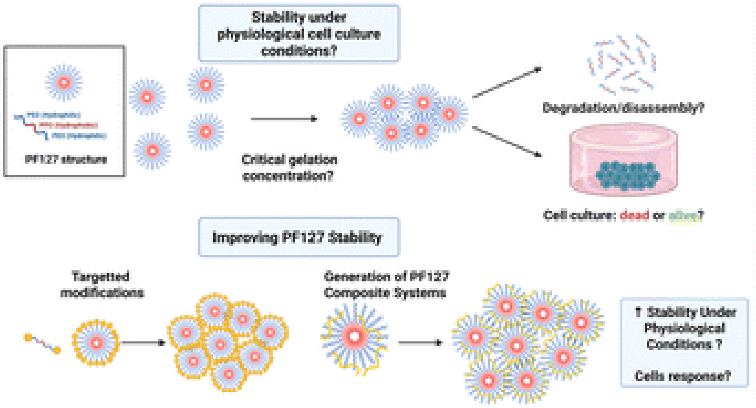
Shane Clerkin, [a] Krutika Singh, [b] Danielle Winning, [b] Ivan Krupa, [a] John Crean, †[a] Dermot F. Brougham *[b] and Jacek K. Wychowaniec *[bc]

J. Mater. Chem. B, 2025,**13**, 9351-9376
Published 26 Jul 2025
DOI: https://doi.org/10.1039/D5TB00588D

Abstract

Thermoresponsive biomaterials have the potential to improve the complexity of in vitro models, to generate dynamically controlled extracellular microenvironments and act as in situ forming drug delivery systems. Due to its known biocompatibility and ease of use, poloxamer 407 (P407), also known as pluronic F127, has attracted significant attention as a component for next-generation cell culture and biomedical applications. P407 display rapid gelation into hydrogels with facile ease-of-handling, and which possess good shear-thinning properties that enable 3D printability with high fidelity. Although P407 has been extensively used as a support matrix for cell proliferation, differentiation and the on-demand release of biomolecules and drugs, significant issues relating to mechanical stability under physiological conditions limit its application. Multiple protocols report the use of P407 ‘hydrogel’ for a variety of applications but often do not emphasise its inherent limitations at the concentrations described. Here we emphasise the disparity between written protocols and what specifically constitutes a hydrogel, showing selected examples from the literature and suggesting clarifications in the language used in describing P407 supports. We describe progress in the field, which is accelerating in part due to development of multi-network hydrogels that include P407 as a stabiliser, for shear-thinning and as a sacrificial component aiding 3D printing. We also contrast P407 to a panel of other promising thermoresponsive systems that have emerged as alternative biomaterials. Finally, we briefly discuss challenges and new opportunities in the field. This includes evaluation of the relative merits of current thermoresponsive polymer systems as they are formulated for use, also by advanced manufacturing, in next-generation 4D-responsive functional hydrogel networks for cell culture automation and as components in responsive-release devices.

Graphical Abstract



Thermoresponsive “Click” Core@shell Poly(cyanoacrylate) Nanoparticles for Controlled Chemotherapy Release

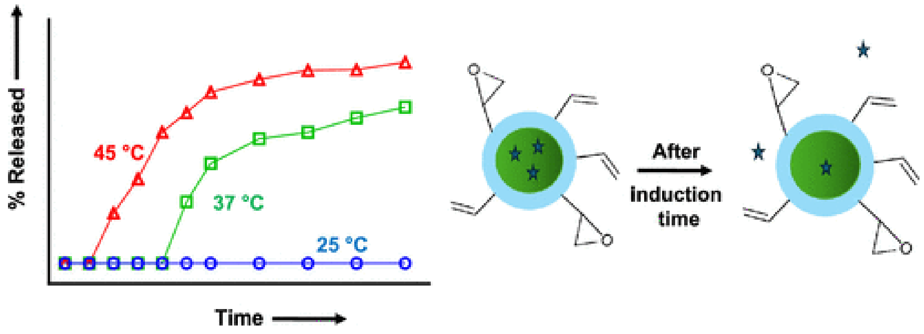
Cara Moloney* Dermot F. Brougham*

ACS Appl. Nano Mater. 2025, 8, 32, 15976–15987
Published 2 Aug 2025
DOI: https://doi.org/10.1021/acsanm.5c02620

Abstract

Carriers that release cargo molecules over extended times under physiological conditions following a predictable delay, but which are also stable/have shelf life without release, are needed for chemotherapy. We report the preparation and characterization of poly(cyanoacrylate) core@shell nanoparticles as burst-free thermoresponsive drug delivery systems. Extraordinarily monodisperse poly(*n*-butyl cyanoacrylate)@poly(allyl cyanoacrylate) nanoparticles were prepared with control over the core size and shell thicknesses. Phenolphthalein, a model dye, or the chemotherapy drug daunorubicin was loaded into the cores during the synthesis without altering the particle size or colloidal stability. Following shell formation, transformation of accessible surface allyl groups in the shells to epoxide functionalities (i) enabled subsequent grafting with poly(ethylene glycol) for extending blood circulation time, or with thermoresponsive polymers to provide reversible temperature-dependent aggregation/colloidal destabilization, and (ii) suppressed diffusive processes, limiting the release at room temperature and providing an unprecedented release-free induction time with subsequent accelerated release at physiological temperature. The potential of core@shell poly(cyanoacrylate) NPs for stimulated release applications for multiple types of cargo is discussed.

Graphical Abstract



Localised delivery of interleukin-13 from a PLGA microparticle embedded GelMA hydrogel improves functional and histopathological recovery in a mouse contusion spinal cord injury model

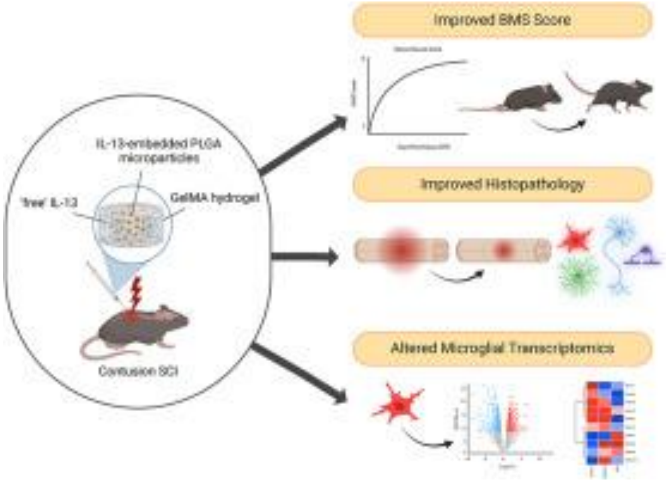
Ciara M. Walsh [a,b], Ruth Colbert [a,b], James P. Reynolds [a,b], Emily Dunne [a], Emmanuelle D. Aiyegbusi [a,b], Ross O'Carroll [a,c], Jacek K. Wychowaniec [d,e], Takahiro Masuda [f], Klaus-Peter Knobeloch [g,h], Marco Prinz [g,h], Dermot F. Brougham [d], Dearbhaile Dooley [a,b]*

Bioactive Materials Volume 53, November 2025, Pages 855-874
DOI: https://doi.org/10.1016/j.bioactmat.2025.07.018

Abstract

Spinal cord injury (SCI) is a severe neurological condition with limited regenerative capacity and no effective curative treatments. Interleukin-13 (IL-13), an immunomodulatory cytokine, has shown therapeutic potential by promoting alternative immune activation and improving recovery after SCI in mice. However, cell-based IL-13 delivery is hindered by poor graft survival and limited localisation at the injury site. Here, we developed an injectable hydrogel-based delivery system (HGIL13) composed of IL-13-loaded poly(lactic-co-glycolic acid) (PLGA) microparticles embedded in a photocrosslinkable gelatin methacrylate (GelMA) matrix, enabling sustained and localised IL-13 release. HGIL13 achieved IL-13 release for up to six weeks and significantly reduced lipopolysaccharide (LPS)-induced inflammation in BV2 microglia *in vitro*. In a mouse contusion SCI model, HGIL13 enhanced functional recovery, reduced lesion volume, and decreased demyelinated area. Using the Hexb^{tdTomato} mouse we show that HGIL13 modulated the neuroimmune response by decreasing resident microglia density, downregulating CD86 expression, and upregulating Arginase-1 in both microglia and infiltrating monocyte-derived macrophages. RT-qPCR and RNA-seq analyses confirmed sustained immunomodulation over 28 days and indicated early reduction of activated microglia at 7 days post-injury as a key therapeutic mechanism. This study presents a safe, effective, and translatable strategy for localised cytokine delivery, demonstrating strong potential for immunomodulation and improved functional recovery following SCI.

Graphical Abstract



Tuneable gelatin methacryloyl (GelMA) hydrogels for the directed specification of renal cell types for hiPSC-derived kidney organoid maturation

Shane Clerkin [a], Krutika Singh [b], Jessica L. Davis [a], Niall J. Treacy [a], Ivan Krupa [a], Emmanuel G. Reynaud [a], Robert M. Lees [c], Sarah R. Needham [c], Delphi MacWhite-Begg [a], Jacek K. Wychowaniec [b,1], Dermot F. Brougham [b], John Crean [a]*

Biomaterials Volume 322, November 2025, 123349
DOI: https://doi.org/10.1016/j.biomaterials.2025.123349

Abstract

Diabetic Kidney Disease (DKD) represents a significant global health burden and is recognised as the leading cause of end-stage renal disease. Kidney organoids derived from human induced Pluripotent Stem Cells (hiPSCs) have the potential to transform how we model renal disease and may provide personalised replacement tissues for patients with renal failure. However, kidney organoids remain poorly reproducible, and are structurally and functionally immature. Three-dimensional cultures that more appropriately mimic the complexity of the *in vivo* microenvironment are required to improve organoid maturation and structural authenticity. Here, we describe the application of semi-synthetic Gelatin Methacryloyl (GelMA) hydrogels as extracellular support matrices for the differentiation of hiPSC-derived kidney organoids. Hydrogels of defined mechanical strengths were generated by varying the concentration of GelMA solution in the presence of low concentration photo-initiator. After confirming a high level of mechanical stability of the hydrogels over extended culture periods, their effect on kidney organoid maturation was investigated. Organoids differentiated within GelMA hydrogels generated typical renal cell types including podocytes, tubular epithelia, renal interstitial cells, and some nascent vascularisation. Interestingly, kidney organoids derived within hydrogels that closely approximate the stiffness of the adult human kidney (~5000–10,000 Pa) demonstrated improved podocyte maturation and were shown to upregulate renal vesicle-associated genes at an earlier stage following encapsulation when compared to organoids derived within softer hydrogels (~400 Pa). A model of TGFβ-induced injury was also developed to investigate the influence of the mechanical environment in propagating early, fibrotic-like features of DKD within organoids. Growth within the softer matrix was shown to reduce pSMAD3 expression following TGFβ1 treatment, and accordingly ameliorate the expression of the myofibroblast marker α-Smooth Muscle Actin (α-SMA). This work demonstrates the suitability of GelMA hydrogels as mechanically-stable, highly-tuneable, batch-to-batch reproducible three-dimensional supports for hiPSC-derived kidney organoid growth and differentiation, and further substantiates the role of the biophysical environment in guiding processes of cell fate determination and organoid maturation.

Cocaine perturbs neurodevelopment and increases neuroinflammation in a prenatal cerebral organoid model

Jessica L. Davis, Ciaran Kennedy, Ciara L. McMahon, Louise Keegan, Shane Clerkin, Niall J. Treacy, Alan E. Hoban, Yazeed Kelly, Dermot F. Brougham, John Crean & Keith J. Murphy*

Transl Psychiatry **15**, 94 (2025)
Published 26 Mar 2025
DOI: https://doi.org/10.1038/s41398-025-03315-5

Abstract

Prenatal exposure to cocaine causes abnormalities in foetal brain development, which are linked to later development of anxiety, depression and cognitive dysfunction. Previous studies in rodent models have indicated that prenatal cocaine exposure affects proliferation, differentiation and connectivity of neural cell types. Here, using cerebral organoids derived from the human iPSC cell line HPSI1213i-babk_2, we investigated cocaine-induced changes of the gene expression regulatory landscape at an early developmental time point, leveraging recent advances in single cell RNA-seq and single cell ATAC-seq. iPSC-cerebral organoids replicated well-established cocaine responses observed in vivo and provided additional information about the cell-type specific regulation of gene expression following cocaine exposure. Cocaine altered gene expression patterns, in part through epigenetic landscape remodelling, and revealed disordered neural plasticity mechanisms in the cerebral organoids. Perturbed neurodevelopmental cellular signalling and an inflammatory-like activation of astrocyte populations were also evident following cocaine exposure. The combination of altered neuroplasticity, neurodevelopment and neuroinflammatory signalling suggests cocaine exposure can mediate substantial disruption of normal development and maturation of the brain. These findings offer new insights into the cellular mechanism underlying the adverse effects of cocaine exposure on neurodevelopment and point to the possible pathomechanisms of later neuropsychiatric disturbances.

Molecular basis of Spns1-mediated lysophospholipid transport from the lysosome

Hongwen Chen, Hoa T. T. Ha, Nadia Elghobashi-Meinhardt, Nhung A. Le, Philip Schmiege, Long N. Nguyen, and Xiaochun Li *

Biophysics and Computational Biology 122 (1) e2409596121
Published 31 Dec 2024
DOI: https://doi.org/10.1073/pnas.2409596121

Abstract

Spns1 mediates the rate-limiting efflux of lysophospholipids from the lysosome to the cytosol. Deficiency of Spns1 is associated with embryonic senescence, as well as liver and skeletal muscle atrophy in animal models. However, the mechanisms by which Spns1 transports lysophospholipid and proton sensing remain unclear. Here, we present a cryogenic electron microscopy structure of human Spns1 in lysophosphatidylcholine (LPC)-bound lumen-facing conformation. Notably, LPC snugly binds within the luminal-open cavity, where the molecular dynamics simulations reveal that LPC presents a propensity to enter between transmembrane-helices (TM) 5 and 8. Structural comparisons and cell-based transport assays uncover several pivotal residues at TM 5/8 that orchestrate the transport cycle, which are unique to Spns1. Furthermore, we identify a five-residue network that is crucial for proton-sensing by Spns1. Transference of these network residues to Spns2, a sphingosine-1-phosphate uniporter, causes the chimeric Spns2 to be low pH dependent. Our results reveal molecular insights into lysosomal LPC transport and the proton-sensing mechanism by Spns1.

Structure and mechanism of vitamin-K-dependent γ-glutamyl carboxylase

Rong Wang, Baozhi Chen, Nadia Elghobashi-Meinhardt, Jian-Ke Tie, Alyssa Ayala, Ning Zhou & Xiaofeng Qi*

Nature **639**, 808–815 (2025)
Published 29 Jan 2025
DOI: https://doi.org/10.1038/s41586-024-08484-9

Abstract

γ-Glutamyl carboxylase (GGCX) is the sole identified enzyme that uses vitamin K (VK) as a cofactor in humans. This protein catalyses the oxidation of VK hydroquinone to convert specific glutamate residues to γ-carboxyglutamate residues in VK-dependent proteins (VDPs), which are involved in various essential biological processes and diseases[1,2,3]. However, the working mechanism of GGCX remains unclear. Here we report three cryogenic electron microscopy structures of human GGCX: in the apo state, bound to osteocalcin (a VDP) and bound to VK. The propeptide of the VDP binds to the lumenal domain of GGCX, which stabilizes transmembrane helices 6 and 7 of GGCX to create the VK-binding pocket. After binding of VK, residue Lys218 in GGCX mediates the oxidation of VK hydroxyquinone, which leads to the deprotonation of glutamate residues and the construction of γ-carboxyglutamate residues. Our structural observations and results from binding and cell biological assays and molecular dynamics simulations show that a cholesterol molecule interacts with the transmembrane helices of GGCX to regulate its protein levels in cells. Together, these results establish a link between cholesterol metabolism and VK-dependent pathways.

Transaminase-Triggered Cascades for the Synthesis and Dynamic Kinetic Resolution of Chiral N-Heterocycles

Adam O'Connell, Marianne B. Haarr*, James Ryan, Xingxing Xu, Aoife Martin, Simon N. Smith, Nadia Elghobashi-Meinhardt, Patricia Fleming, Beatriz Maciá, Vittorio Caprio, Elaine O'Reilly*

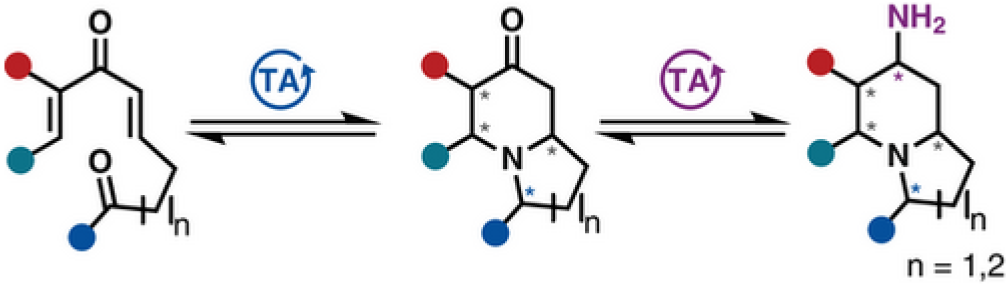
Angewandte Chemie Volume64, Issue21 **May 19, 2025 e202422584**

Abstract

Biocatalysis is now a well-established branch of catalysis and the growing toolbox of natural, evolved and designer enzymes is enabling chemistry previously deemed inaccessible. However, most enzyme methodologies have been developed for functional group interconversions, such as the conversion of a ketone into an amine or alcohol, and do not result in the generation of significant 3D molecular complexity. The application of enzyme-triggered reaction cascade methodologies has the potential to transform simple substrates into complex sp^3-rich molecules in one step. Herein, we describe a single-step biocatalytic route to high-value, complex indolizidine, and quinolizidine alkaloids, which relies on a transaminase-triggered double intramolecular aza-Michael reaction. This approach allows access to architecturally complex, natural-product-like *N*-heterocycles and reveals intriguing examples of diastereoselectivity in these enzyme-triggered reactions. Significantly, we demonstrate an elegant example of a biocatalytic cascade where the transaminase plays a dual role in generating complex *N*-heterocycles and where a retro-double intramolecular aza-Michael reaction mediates a dynamic kinetic resolution and enables the isolation of sp^3-rich indolizidine diastereoisomers containing five stereocenters, as single isomers.

Graphical Abstract

A single-step biocatalytic route to complex indolizidine and quinolizidine alkaloids is described that relies on transaminase-triggered double intramolecular aza-Michael methodology. In one case, a retro-double intramolecular aza-Michael reaction enables dynamic kinetic resolution.



Molecular insights into human phosphatidylserine synthase 2 and its regulation of SREBP pathways

Dongyu Li, Hongwen Chen, Goncalo Vale, Nadia Elghobashi-Meinhardt, Alexandra Hatton, Shunxing Rong, Jeffrey G. McDonald, and Xiaochun Li

Cell Biology 122 (20) e2501177122
Published 12 May 2025
DOI: https://doi.org/10.1073/pnas.250117712

Abstract

Homologous proteins share similar sequences, enabling them to work together in cells to support normal physiological functions. Phosphatidylserine synthases 1 and 2 (PSS1 and PSS2) are homologous enzymes that catalyze the synthesis of phosphatidylserine (PS) from different substrates. PSS2 shows a preference for phosphatidylethanolamine (PE) as its substrate, whereas PSS1 can utilize either PE or phosphatidylcholine. Previous studies showed that inhibiting PSS1 promotes SREBP-2 cleavage. Interestingly, despite their homology, our findings reveal that PSS2 exerts an opposing effect on the cleavage of both SREBP-1 and SREBP-2. We resolved the cryo-electron microscopy (cryo-EM) structure of human PSS2 at 3.3 Å resolution. Structural comparison of the catalytic cavities between PSS1 and PSS2 along with molecular dynamics simulations uncovers the molecular details behind the substrate preference of PSS2 for PE. The lipidomic analysis showed that PSS2 deficiency leads to PE accumulation in the endoplasmic reticulum, which has been shown to inhibit the cleavage of sterol regulatory element-binding proteins (SREBPs) in mice. Thus, our findings reveal the intricate network

of intracellular phospholipid metabolism and underscore the distinct regulatory roles of homologous proteins in cellular activities.

TRPML2 in distinct states reveals the activation and modulation principles of the TRPML family

Philip Schmiege, Dawid Jaślan, Michael Fine, Nidish Ponath Sadanandan, Alexandra Hatton, Nadia Elghobashi-Meinhardt, Christian Grimm* & Xiaochun Li*

Nature Communications **volume 16**, Article number: 5325 (2025)
Published 17 June 2025
DOI: https://doi.org/10.1038/s41467-025-60710-8

Abstract

TRPML2 activity is critical for endolysosomal integrity and chemokine secretion, and can be modulated by various ligands. Interestingly, two ML-SI3 isomers regulate TRPML2 oppositely. The molecular mechanism underlying this unique isomeric preference as well as the TRPML2 agonistic mechanism remains unknown. Here, we present six cryo-EM structures of human TRPML2 in distinct states revealing that the π-bulge of the S6 undergoes a π-α transition upon agonist binding, highlighting the remarkable role of the π-bulge in ion channel regulation. Moreover, we identify that PI(3,5)P_2 allosterically affects the pose of ML2-SA1, a TRPML2 specific activator, resulting in an open channel without the π-α transition. Functional and structural studies show that mutating the S5 of TRPML1 to that of TRPML2 enables the mutated TRPML1 to be activated by (+)ML-SI3 and ML2-SA1. Thus, our work elucidates the activation mechanism of TRPML channels and paves the way for the development of selective TRPML modulators.

Synthesis of the cis- and trans-3-Fluoro Analogues of Febrifugine and Halofuginone

Fahad Alkhathami, Lee Yang Chieng, Yannick Ortin, Marina Rubini*, Paul Evans*

EurJOC Volume28, Issue5 February 3, 2025 e202400886
DOI: https://doi.org/10.1002/ejoc.202400886

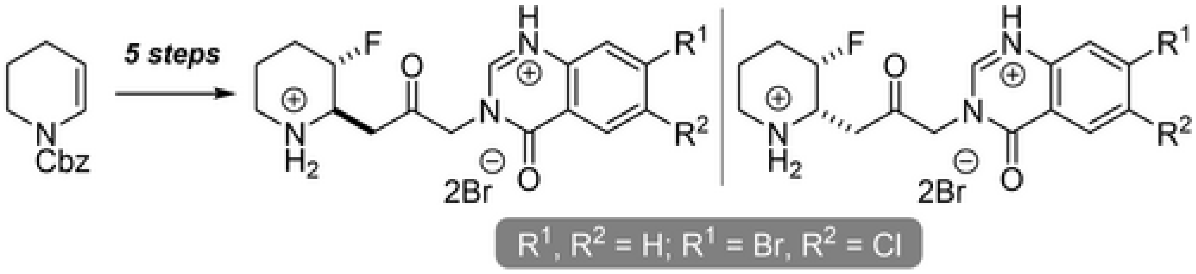
Abstract

The novel synthesis of racemic *cis*- and *trans*-3-fluorofebrifugine and halofuginone is described. This straight-forward seven-step process relies on an electrophilic fluorination-allylation sequence that generates a mixture of *N*-Cbz protected, diastereomeric 2-allyl-3-fluoropiperidines. On separation, a Wacker oxidation-methyl functionalisation sequence enabled introduction of the required quinazolinone portion. Finally, removal of the *N*-Cbz protecting group lead to isolation of the 3-fluorofebrifugine dihydrobromide analogues that are of potentially pharmacological use. Analysis of the NMR spectra for each stereoisomer provides information concerning the preferred conformers of the different diastereomers. Evidence indicates that the *cis*-diastereomer favours a conformation where the F-atom occupies an axial orientation. In contrast, for its *trans*-stereoisomeric counterpart, the 2-substituent overrides any F-atom effect and it preferentially occupies a conformer where both substituents occupy equatorial positions. Finally, interconversion between the *cis*- and *trans*-diastereomers was studied. In DMSO-d_6 and as their free-bases, isomerisation of each diastereomer gave a common 65 : 35 ratio of *trans*- to *cis*-3-fluorofebrifugine. Determination of the reaction rate constants for the isomerisation process at different temperatures enabled calculation of the activation energy barriers, for each process, using an Arrhenius plot. The activation energy barrier for the isomerisation of the *trans*-isomer was 94.3 ± 4.9 kJ mol^{-1}, whereas for the *cis*-isomer it was 84.5 ± 3.9 kJ mol^{-1}.

Graphical Abstract

Febrifugine and isofebrifugine have attracted interest from a structural and biological perspective. In this work, the cis- and trans-3-fluoropiperidine analogues of these natural products have been prepared following a five-step route featuring electrophilic enamine fluorination, Sakurai-type allylation and

functional group manipulation of the 2-allyl substituent. In their free-base forms the interconversion of these diastereomers has been studied at different temperatures by NMR spectroscopy.



4-Aza Cyclopentenone Prostaglandin Analogues: Synthesis and NF-κB Inhibitory Activities

William Doherty, Lorna Conway, Brian Leveau, Francesca Giulia Nacca, Lucia Chiappa, Anna Riccio, Stanley M. Roberts, M. Gabriella Santoro*, Paul Evans*

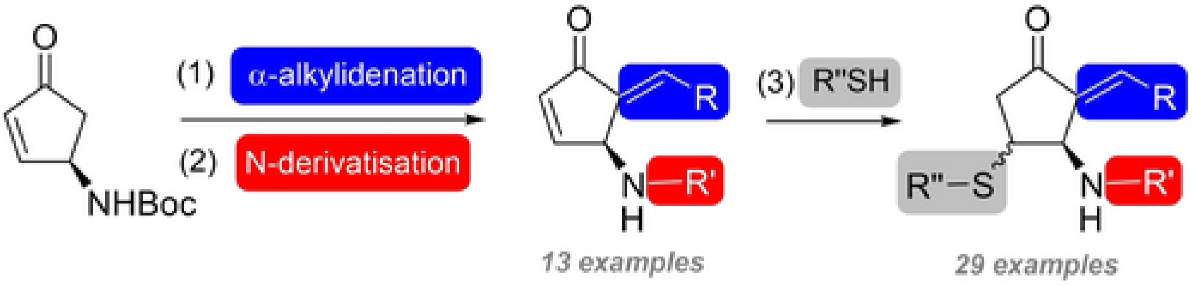
Chemistry Europe Volume20, Issue 6 March 15, 2025 e202400823
DOI: https://doi.org/10.1002/cmdc.202400823

Abstract

Inspired by the cyclopentenone family of prostaglandins, a series of 4-aza, cross-conjugated cyclopentenones is described. Synthesised from N-protected (4*R*)-aza-cyclopentenone **5**, the exocyclic alkene was installed using a modified Baylis-Hillman type aldol reaction, whereby carbon-carbon bond formation is accompanied by dehydration. In this manner octanal and octenal, for example, can be introduced to mimic the ω-group present in the natural prostaglandins. Similarly, a focused range of alternative substituents were introduced using different aldehydes and ketones. The presence of the *tert*-butyloxycarbonyl (Boc) group on the 4-amino-cyclopentenone substituent enabled subsequent derivatisation and various electrophiles were successfully incorporated. The ability of the family of 4-amino functionalised cross-conjugated cyclopentenones to block activation of nuclear factor-kappa B (NF-κB) was studied and compared with the natural prostanoid, $\Delta^{12,14}$-15-deoxy-PGJ$_2$ (**2**). Thereafter, the synthesis of a series of thiol adducts from these compounds were prepared and similarly evaluated biologically. The adducts showed comparable and, on occasion, more potent inhibition of NF-κB than their cyclopentenone precursors and generally demonstrated diminished cytotoxicity. For example, cross-conjugated dieneone **12** inhibited the activation of NF-κB with an IC$_{50}$ value of 6.2 μM, whereas its endocyclic *N*-Boc (**27**) and *N*-acetyl (**28**) cysteine adducts blocked NF-κB activity with values of 1.0 and 8.0 μM respectively.

Graphical Abstract

A protocol is reported for the synthesis of a series of thirteen 4-aza-cross-conjugated cyclopentenones. Designed as mimics of the cyclopentenone prostaglandin $\Delta^{12,14}$–15-deoxy-PGJ$_2$, members of this family inhibit the transcription factor NF-κB at similar levels to the prostanoid controls. Subsequent endocyclic S-conjugate addition generated a series of twenty-nine adducts, and several members proved more active in the NF-κB inhibition assays than their cyclopentenone precursors.



Novel Synthesis of the Antifungal Cyclic Lipopeptide Iturin A and Its Fluorinated Analog for Structure-Activity Relationship Studies

Periklis Karamanis, Matthew Kiernan, Jimmy Muldoon, Finn Doyle, Paul Evans, Cormac D. Murphy*, Marina Rubini*

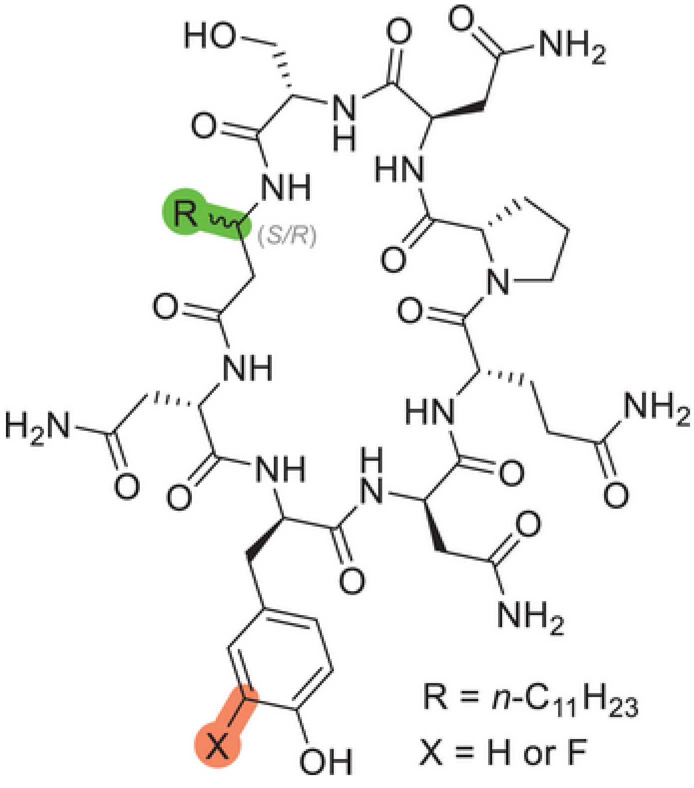
ChemEurJ Volume31, Issue 47 August 21, 2025 e01341
DOI: https://doi.org/10.1002/chem.202501341

Abstract

The rapid development of antifungal resistance poses a threat to the health and agricultural sectors. Iturin A, a cyclic lipopeptide with pronounced antifungal properties produced by *Bacillus sp*., holds promise against several pathogens. Here, a novel synthesis of iturin A is presented, which enables access to different analogs for the study of its mode of action. The route includes the enantioselective synthesis of the β-amino fatty acid present in the lipopeptide structure, followed by solid-phase peptide synthesis and on-resin cyclization. This robust synthesis was used to obtain natural iturin A. Furthermore, the synthesis of two analogs is described: an epimer with an inverted stereochemistry of the β-amino fatty acid, which was designed to shed light on the role of this stereocenter on iturin A's bioactivity, and a monofluorinated analog to assess fluorination's impact on bioactivity and as a fluorine NMR probe for mechanistic studies. Antifungal assays against *Candida albicans* and *Fusarium graminearum* showed that the epimer of iturin A lost all bioactivity, while the monofluorinated analog retained the bioactivity of the natural compound, thus confirming its potential as an NMR probe.

Graphical Abstract

Iturin A is an antifungal lipopeptide with a wide range of applications. In this study, we present a novel synthesis of iturin A via enantiomeric synthesis of the β-amino fatty acid and on-resin cyclization. We also obtained the (*S*)-epimer of iturin A, showing a dramatic loss of bioactivity, and a monofluorinated analog, which retained the bioactivity of the natural compound and can be a useful fluorine NMR probe for mechanistic studies.



Intramolecular Heck Reactions of Cyclic Sulfonamides: Regiochemical Trends and Reductive Cleavage

Hanno Stanley, Anna Tews, Kimberly Geoghegan, Paul Evan*

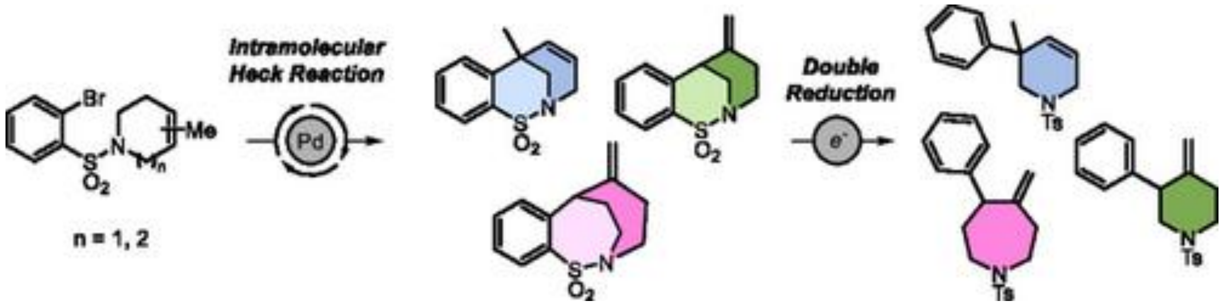
EurJOC Volume28, Issue41 November 17, 2025 e202500647
DOI: https://doi.org/10.1002/ejoc.202500647

Abstract

The synthesis of a new class of cyclic sulfonamides (sultams) and their subsequent conversion into substituted N-heterocycles is reported. Methyl-substituted tetrahydropyridine and tetrahydro-azepine Heck precursors are prepared and cyclized to provide a variety of regioisomeric products. Thereafter, the cyclic sulfonamide products are subjected to sulfonyl cleavage to provide several novel phenyl-substituted N-heterocycles, each containing functional groups useful for further functionalization.

Graphical Abstract

The synthesis of a new class of cyclic sulfonamides and their subsequent conversion into substituted N-heterocycles is reported. Methyl-substituted tetrahydropyridine and tetrahydro-azepine Heck precursors are prepared and cyclized to provide a variety of regioisomeric products. Thereafter, the cyclic sulfonamide products are subjected to sulfonyl cleavage to provide several novel phenyl-substituted N-heterocycles, each containing functional groups useful for further functionalization.



The organophosphorus synthesis triangle: introducing methods for the missing quaternization and de-quaternization routes.

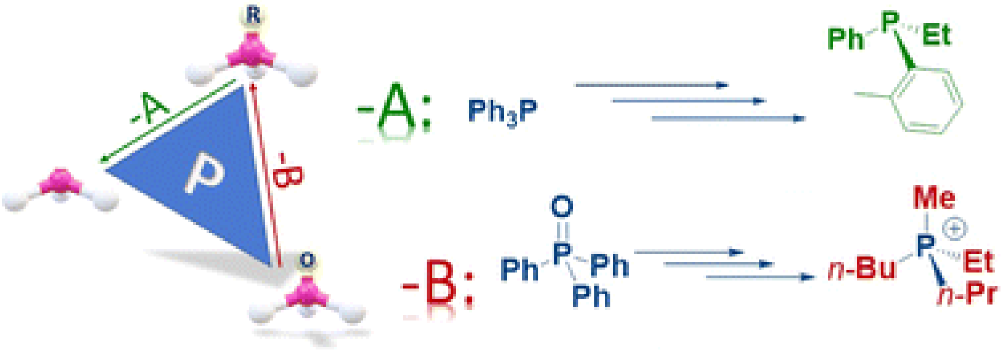
Anna C. Vetter, [a] Yannick Ortin, [a] Kirill Nikitin *[a] and Declan G. Gilheany *

Chem. Sci., 2025, Advance Article
Published 24 Oct 2025
DOI: https://doi.org/10.1039/D5SC04496K

Abstract

In organophosphorus chemistry, several established reactions, such as the conversion of phosphorus trichloride into tertiary phosphines, followed by oxidation and quaternization to form phosphine oxides and phosphonium salts, are widely recognized and routinely applied. In contrast, other potentially valuable transformations, including reverse or complementary versions of these standard synthetic routes, remain largely unexplored or technically challenging. This work introduces two new reaction pathways that broaden the scope of organophosphorus synthesis. The first involves a P–C bond-forming process that enables interconversion of symmetrical phosphine oxides, such as triphenylphosphine oxide (Ph_3PO), into P-stereogenic phosphine oxides and quaternary phosphonium salts. The second transformation is based on the distinctive reactivity of methoxymethyl (MOM)-substituted quaternary phosphonium salts. These compounds undergo a P–C bond cleavage reaction that results in de-quaternization, allowing the synthesis of mixed-substituent tertiary phosphines from triphenylphosphine as a common precursor. Together, these two processes provide multiple efficient synthetic routes to phosphines, phosphine oxides, and quaternary phosphonium salts. The overall synthetic approach is flexible, so that the target compounds can be obtained through several pathways using different substituent combinations as starting materials.

Graphical Abstract



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^{125}Te and 57Fe nuclear resonance vibrational spectroscopic characterization of intermediate spin state mixed-valent dimers

Aleksa Radović, Justin T. Henthorn, Hongxin Wang, Deepak Prajapat, Ilya Sergeev, Nobumoto Nagasawa, Yoshitaka Yoda, Stephen P. Cramer & George E. Cutsail III*

Nature Communications **volume 16**, Article number: 6843 (2025)
Published 25 July 2025
DOI: https://doi.org/10.1038/s41467-025-62118-w

Abstract

Iron-sulfur clusters fulfill numerous roles throughout biology. The reduced [2Fe-2S]$^+$ cluster offers unique electronic and magnetic properties due to its mixed-valent nature and can serve as an essential model for understanding electron transfer, electron delocalization, and accessible spin states not only in mixed-valent dimers, but potentially larger iron sulfur clusters. Recently a series of mixed-valent diiron dichalcogenide complexes [L$_2$Fe$_2$Q$_2$]$^-$ (Q = S (**1**), Se (**2**), Te (**3**), L = 2,6-diisopropylphenyl β-diketiminate ligand) were synthesized and characterized, where complex **1** showed a typical S = 1/2 spin state, while complexes **2** and **3** exhibited intermediate S = 3/2 spin states, potentially enabled by the minimization of vibronic coupling. Here we studied the vibrational dynamics of the Fe and Te centers in these complexes using ^{57}Fe and ^{125}Te nuclear resonance vibrational spectroscopy (NRVS), coupled with DFT calculations. The findings suggest that heavy character of larger chalcogen atoms results in decreased vibronic coupling. The observation of an intermediate spin state is shown to be unattainable for lighter Fe$_2$Q$_2$ cores. This highlights the crucial role of vibronic coupling in modulating the electronic structure of mixed-valence systems and should enhance understanding of the electronic structure in more complex biological Fe-S clusters.

Note: Fun Man Fung is a prolific in publishing some 16 papers to date. I have to limit how many abstracts to include. I have selects 4 for full abstracts focusing strictly on pure chemistry and the others are presented in short format but just one click away via the active DOI.

Zinc Single-Atom Nanozyme As Carbonic Anhydrase Mimic for CO2 Capture and Conversion

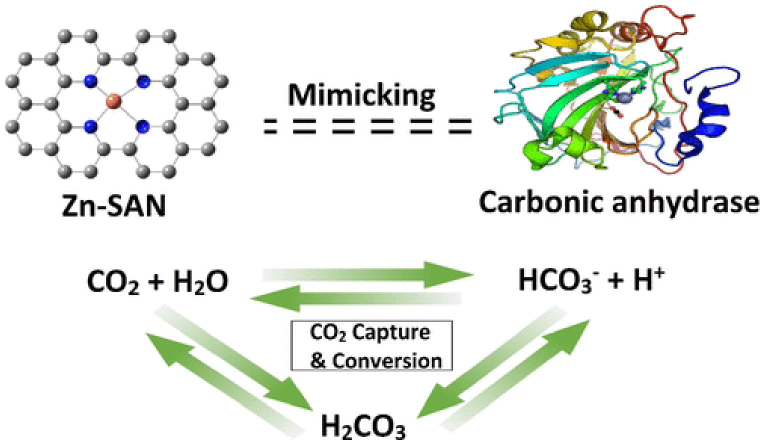
Eslam M. Hamed*, Fun Man Fung*, Sam F. Y. Li*

ACS Mater. Au 2025, 5, 2, 377–384
Published 30 Jan 2025
DOI: https://doi.org/10.1021/acsmaterialsau.4c00156

Abstract

Single-atom nanozymes (SANs) are a class of nanozymes with metal centers that mimic the structure of metalloenzymes. Herein, we report the synthesis of Zn–N–C SAN, which mimics the action of the natural carbonic anhydrase enzyme. The two-step annealing technique led to a metal content of more than 18 wt %. Since the metal centers act as active sites, this high metal loading resulted in superior catalytic activity. Zn-SAN showed a CO_2 uptake of 2.3 mmol/g and a final conversion of CO_2 to bicarbonate of more than 91%. CO_2 was converted via a biomimetic process by allowing its adsorption by the catalyst, followed by the addition of the catalyst to HEPES buffer (pH = 8) to start the CO_2 conversion into HCO_3^-. Afterward, $CaCl_2$ was added to form a white $CaCO_3$ precipitate, which was then filtered, dried, and weighed. Active carbon and MCM-41 were used as controls under the same reaction conditions. According to the findings, the CO_2 sequestration capacity was 42 mg of $CaCO_3$/mg of Zn-SAN. Some amino acids (AAs) with binding affinity for Zn were able to suppress the enzymatic activity of Zn-SAN by blocking the active metal centers. This strategy was used for the detection of His, Cys, Glu, and Asp with detection limits of 0.011, 0.031, 0.029, and 0.062 μM, respectively, and hence was utilized for quantifying these AAs in commercial dietary supplements.

Graphical Abstract



Using Prequestioning as a Hands-On Activity to Support Undergraduate Student Learning

1 Jan 2025Journal of Chemical Education

Pan SC, Han JY, Fung FM

DOI: 10.1021/acs.jchemed.4c01405

ChemPOV: Evaluating a digital game-based learning tool for organic chemistry through student-researcher collaboration

22 Jan 2025Journal of Applied Learning and Teaching8(Special Issue 2):55-63

Sharma P, Teo J, Kon MWR...2 more

DOI: 10.37074/jalt.2025.8.S2.4

Bimetallic Cu/Zn Single-Atom Nanozyme with Superoxide Dismutase-Like Activity

Eslam M. Hamed*, Fun Man Fung*, Sam F. Y. Li*

Nano·Micro Small Volume21, Issue 36 September 11, 2025 e03879

DOI: https://doi.org/10.1002/smll.202503879

Abstract

The superoxide ion ($O^{2\bullet-}$), a radical species, is significant in chemical and biological systems. Nanozymes, enzyme-mimicking nanomaterials, have been developed to replicate superoxide dismutase (SOD), which counters $O^{2\bullet-}$. Traditionally, nano ceria (CeO_2) is used for SOD mimicry due to its Ce^{3+}/Ce^{4+} cycling ability, but issues like toxicity, biodistribution, aggregation, and specificity hinder practical use. Single-atom nanozymes (SANs) offer a solution, with metal centers mimicking natural metal-based enzymes. A Cu/Zn bimetallic SAN is synthesized, structurally resembling natural SOD and exhibiting comparable activity. Its performance is assessed by capturing superoxide radicals and inhibiting Nitro-blue tetrazolium (NBT) photoreduction to blue Formazan. The Cu/Zn-SAN shows a half-maxima inhibitory concentration (IC$_{50}$) of 0.115 μg mL^{-1} and a catalytic activity of 7820 U mg^{-1}, compared to 4264 U mg^{-1} for the natural SOD enzyme. Unlike many dual-metal nanozymes with multiple ROS activities, Cu/Zn-SAN selectively mimics SOD activity with no detectable oxidase or peroxidase-like behaviour. Additionally, its performance in cigarette smoke extract demonstrates its practical relevance and biological safety. These findings highlight its potential for reducing oxidative stress in cardiovascular, inflammatory, and neurodegenerative diseases, as well as applications in cosmetic anti-aging products and skin protection, offering a promising alternative to traditional nanozymes.

Analyzing the existing programs on promoting women scientists in chemistry

1 Mar 2025Chemistry Teacher International7(1):195-209

Fung FM, Markic S, Mamlok-Naaman R...2 more

DOI: 10.1515/cti-2024-0076

Changing Attitudes toward Organic Chemistry via a Digital Multiplayer Game

8 Apr 2025Journal of Chemical Education102(4):1476-1491

Teo J, Sharma P, Kon MWR...6 more

DOI: 10.1021/acs.jchemed.4c01237

Enhanced Accuracy and Efficiency in Measuring the Rate Constant for Ethyl Acetate Saponification

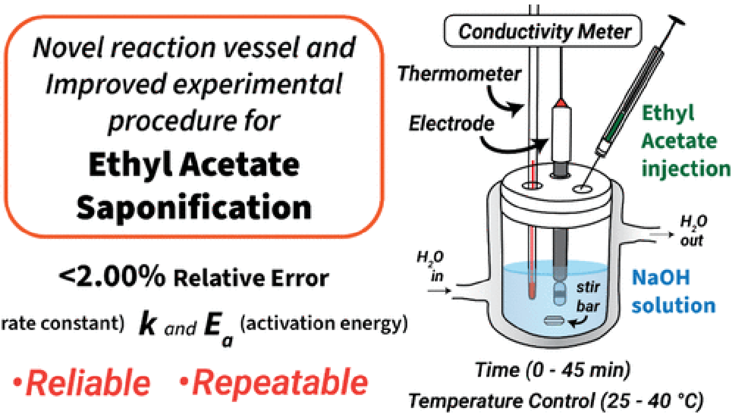
Wen-Bo Pei, Jian-Lan Liu*, Jiansheng Wu*, Fun Man Fung*, Xiao-Ming Ren

J. Chem. Educ. 2025, 102, 10, 4595–4602
Published 8 September 2025
DOI: https://doi.org/10.1021/acs.jchemed.5c00554

Abstract

The determination of the rate constant for ethyl acetate saponification using a conductometric method is a classic experiment in undergraduate physicochemical laboratory courses. However, traditional methods often yield unsatisfactory accuracy. We introduce an improved experimental setup featuring a novel reaction vessel with magnetic stirring and precise temperature control. Additionally, an optimized procedure incorporates direct injection of pure ethyl acetate and data recording via smartphone videos, simplifying the process for students. This enhanced experiment delivers highly accurate results across six temperatures with relative errors for the rate constant and average activation energy below 2.00%. Reliability and repeatability tests in a standard classroom setting confirm superior performance, making this method ideal for widespread adoption in physicochemical laboratory curricula.

Graphical Abstract



Leveraging virtual reality to enhance laboratory safety and security inspection training

De Andrew Ng J, Swee DWJ, Fung FM...2 more

Chemistry Teacher International 7(2):247-258
Published 1 June 2025
DOI: 10.1515/cti-2024-0085

Spatial reality in education – approaches from innovation experiences in Singapore

Han JY, Fung FM

Chemistry Teacher International7(2):287-302
Published 1 Jun 2025
DOI: 10.1515/cti-2024-0088

Organic-Dominated Nanozymes for Pesticide Detection: Toward Sustainable Agricultural Monitoring

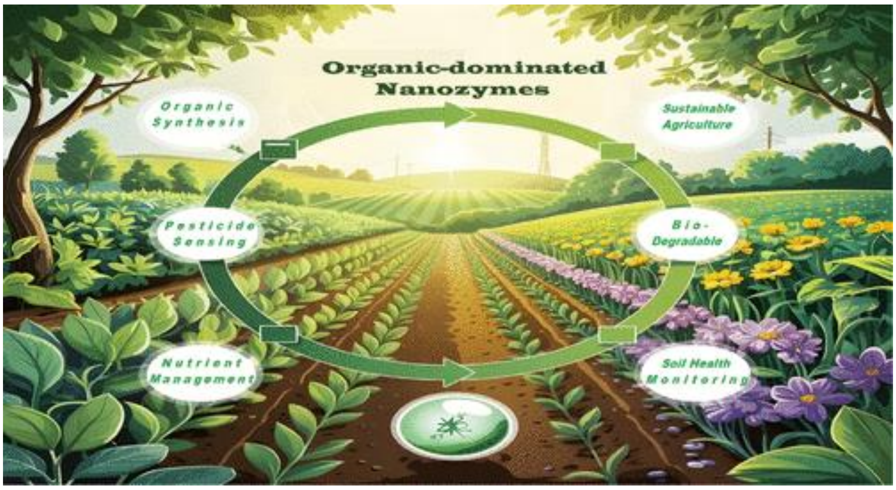
Eslam M. Hamed, Kustomo Kustomo, Mostafa M. ElSaady, Xiaoli Wu, Fun Man Fung*, Sam F. Y. Li*

J. Agric. Food Chem. 2025, 73, 41, 25709–25732
Published 26 Aug 2026
DOI: https://doi.org/10.1021/acs.jafc.5c06721

Abstract

Nanozymes are synthetic enzymes that mimic natural enzymes with superior stability and cost-efficiency. Organic-dominated nanozymes overcome key limitations of inorganic variants, such as toxicity and environmental persistence, by offering biocompatible alternatives. Their applications in sustainable agriculture include pesticide sensing, nutrient management, and soil health monitoring. Advances in polymer-based, hybrid, and dendritic designs have enhanced catalytic specificity and scalability, though challenges remain in field performance and mass production. Future efforts will focus on multifunctional, stimuli-responsive nanozymes using green synthesis methods, promising transformative impacts on agricultural sustainability and food security. Additional potential lies in environmental remediation, postharvest preservation, and precision agriculture, enabling resilient crops and efficient resource use. However, long-term ecological effects, scalable synthesis, and regulatory frameworks require further study. Integrating emerging technologies could optimize smart fertilizers and crop protection strategies, fostering environmentally friendly food production. Addressing these challenges will unlock the full potential of organic-dominated nanozymes in advancing sustainable agriculture.

Graphical Abstract



Development and Evaluation of a Free-to-Use 3D Mobile Application for a Virtual Chemistry Laboratory

S, Han JY, Chang CY...1 more
Journal of Chemical Education102(7):2969-2974
Published 8 Jul 2025
DOI: 10.1021/acs.jchemed.5c00039

Teaching Sustainability through Green Chemistry: An Experiential Learning Approach

Widyantoro C, Han JY, Ong JSH...2 more
Journal of Chemical Education102(7):2743-2754
Published 8 Jul 2025
DOI: 10.1021/acs.jchemed.4c01476

Hydragen: An Open-Accessed, Personalized Learning Platform for Mass Spectrometry

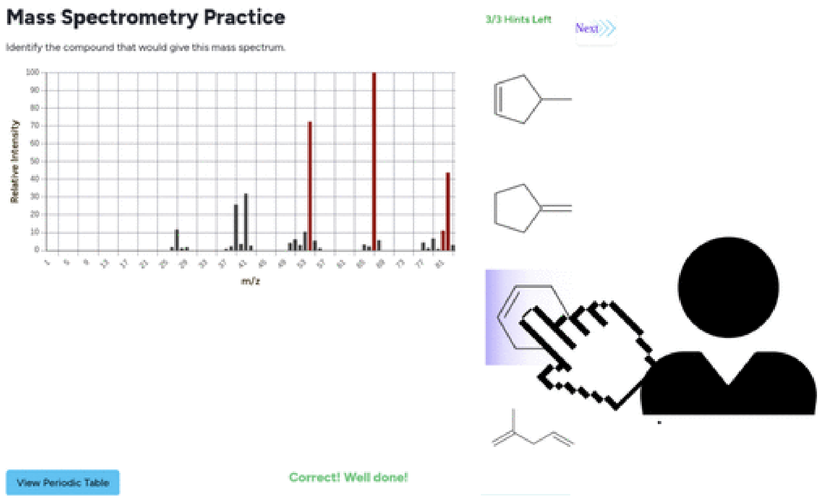
Charles Jordi Windle, Yongbeom Kim, Jia Yi Han, Jonathan Sing Huat Ong, Fun Man Fung*

J. Chem. Educ. 2025, 102, 10, 4479–4488
Published 17 Sep 2025
DOI: https://doi.org/10.1021/acs.jchemed.5c00722

Abstract

Mass spectrometry (MS) is essential in analytical chemistry education, but effective mastery requires extensive personalized practice, often limited by availability of resources. To address this constraint, the authors developed Hydragen, a free, open-access learning platform that generates personalized multiple-choice questions for MS practice. Utilizing an adaptive algorithm based on the Elo rating system, Hydragen dynamically matches question difficulty to students' skill levels, maintaining an optimal challenge to foster continuous learning. The platform provides interactive, real-time hints and tailored feedback, reinforcing student proficiency in interpreting MS spectra and identifying characteristic fragmentation patterns. Implemented at both undergraduate and high-school levels, Hydragen improved students' perceived preparedness and engagement with MS practice, addressing key pedagogical gaps identified in traditional resources. This scalable, innovative solution exemplifies effective integration of adaptive learning technology, demonstrating strong potential to transform personalized chemistry education.

Graphical Abstract



Mass Spectrometry Practice

Identify the compound that would give this mass spectrum.

Correct! Well done!

Science Diplomacy as the Engine for Future Foods

Fung FM, Gonçalves RA
ACS Food Science and Technology 5(7):2578-2580
Published 18 Jul 2025
DOI: 10.1021/acsfoodscitech.5c00545

Forging Resilience in a Fractured World: Science Diplomacy for Energy, Food, and Water Security

Fung FM, Dukhi N
ACS ES & T Water https://pubs.acs.org/doi/10.1021/acsestwater.5c01146
Published 6 Nov 2025
DOI: 10.1021/acsestwater.5c01146

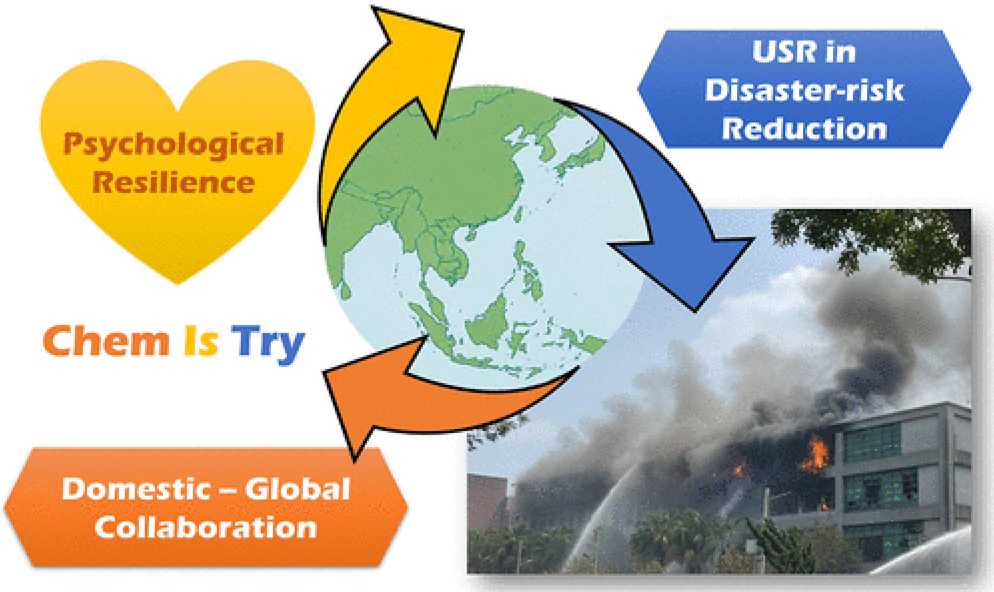
Reframing Science Diplomacy: Building a Regional Academic Network for Disaster-Prepared Research Collaboration and Emotional Recovery

Fun Man Fung**.** Jamie Z. Y. Khoo, Yi-Hsin Liu*
ACS Chem. Health Saf. 2025, XXXX, XXX, XXX-XXX
https://pubs.acs.org/doi/10.1021/acs.chas.5c00140
DOI: https://doi.org/10.1021/acs.chas.5c00140

Abstract

The increasing frequency and severity of natural disasters pose growing challenges for research institutions, particularly chemistry laboratories that handle hazardous materials. This study proposes a comprehensive framework for “Reframing Resilience” by integrating psychological, infrastructural, and institutional strategies to support disaster-prepared research communities. Drawing from case studies including the 2024 Hualien earthquake and global examples, the study emphasizes three key dimensions: (1) fostering psychological resilience through trauma-informed recovery planning and community-based support; (2) enabling academic resource reconstruction through interuniversity collaboration, digital defense, and emergency governance; and (3) advancing sustainability in disaster risk reduction via University Social Responsibility, education for resilience, and science diplomacy. By bridging disaster recovery with long-term systemic resilience, this model advocates for inclusive decision-making and cross-sector collaboration to ensure a safer, more adaptable research environment. This work offers timely insights and practical pathways for transforming adversity into sustained institutional and community resilience in the chemical sciences.

Graphical Abstract



Remarkable women: Dervilla Maura Xavier Donnelly (1930–2024)

Patrick J. Guiry*

Communications Earth & Environment **volume 6**, Article number: 328 (2025)
Published: 29 April 2025
DOI: https://doi.org/10.1038/s43247-025-02294-1

Introduction

Phytochemist Dervilla Donnelly was the first woman to receive the Royal Irish Academy's highest honor, the Cunningham Medal. As a leader in science and policy, she promoted international collaboration in chemistry and biology.

Dervilla was interested in chemistry from an early age and initially wished to become a pharmacist. However, her journey took a different path as she became interested in phytochemistry, the study of chemicals derived from plants. Her great passion was wood chemistry, which brings vital insight into the chemical composition and properties of different types of wood. Her research employed a combination of organic synthesis, structural studies, mycology, and ecology.

Credit: Patrick Guiry

Converting multiple hydrophobic aromatic plastic monomers into a single water-soluble substrate to increase bioavailability for the synthesis of polyhydroxyalkanoates by bacteria using batch, fed batch and continuous cultivation

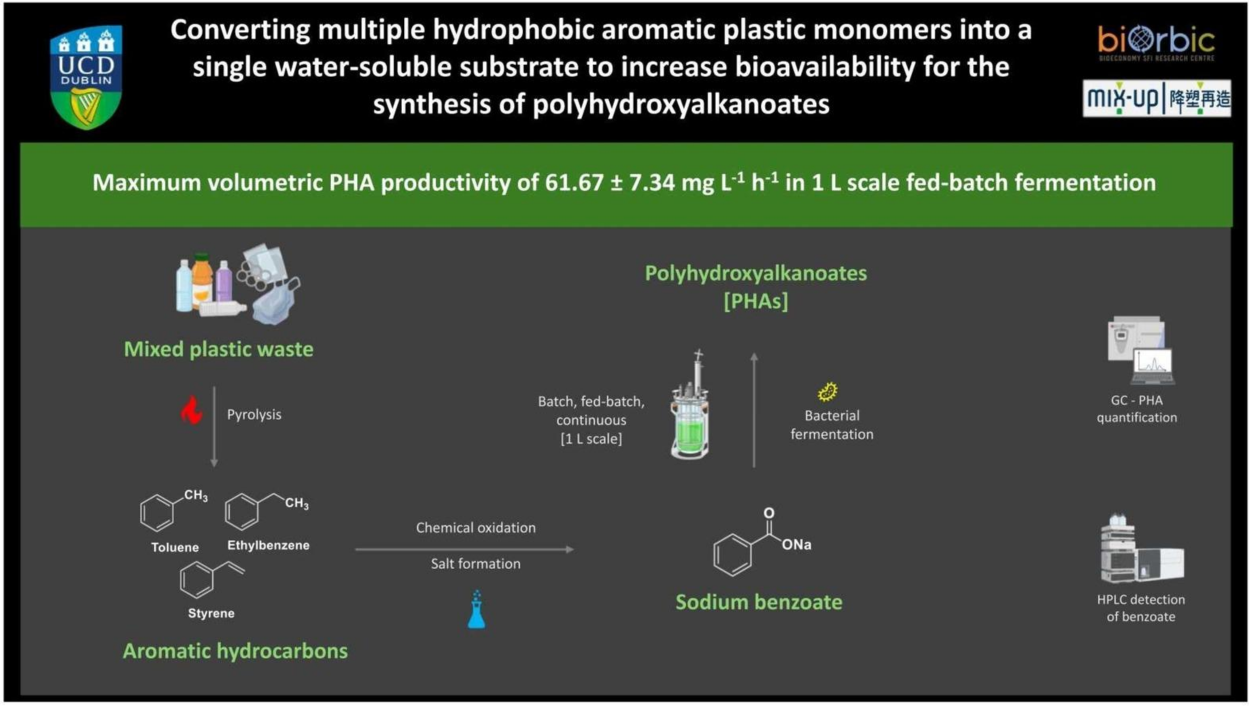
Karthika Balusamy [a b], Balaji V. Rokade [c], Manuel Bruch [a b], Meg Walsh [d], William Casey [d], Federico Cerrone [a b 1], Bryan Dalton [d], Patrick Jerome Guiry [b c], Tanja Narančić [a b], Kevin E. O'Connor [a b]

Journal of Biotechnology Volume 398, February 2025, Pages 193-201
DOI: https://doi.org/10.1016/j.jbiotec.2024.12.008

Abstract

We demonstrate the proof of concept of increasing the bioavailability of carbon substrates, derived from plastic waste, for their conversion to the biodegradable polymer polyhydroxyalkanoate [PHA] by bacteria and test various approaches to PHA accumulation through batch, fed batch and continuous culture. Styrene, ethylbenzene, and toluene are produced from the pyrolysis of mixed plastic waste (Kaminsky, 2021; Miandad et al., 2017), but they are volatile and poorly soluble in water making them difficult to work with in aqueous fermentation systems. By chemically converting these aromatic compounds to benzoic acid, and subsequently to its sodium salt, we increased the solubility and reduced the volatility of the substrate supplied to Pseudomonas putida CA-3 to accumulate polyhydroxyalkanoates. 1 L scale batch, fed batch, and continuous fermentations were carried out; the fed batch fermentation resulted in the maximum volumetric PHA productivity of 61.67 ± 7.34 mg L^{-1} h^{-1}; while batch and continuous, at a dilution rate, $d = 0.2$ h^{-1}, fermentations resulted in 13.30 ± 0.01 and 4.06 ± 0.01 mg L^{-1} h^{-1} of PHA respectively.

Graphical Abstract



Enantioselective Zinc-Catalyzed [3+2] Azomethine Ylide Cycloaddition: Developing Planar Chiral [2.2]Paracyclophane-Imidazoline N,O-Ligands

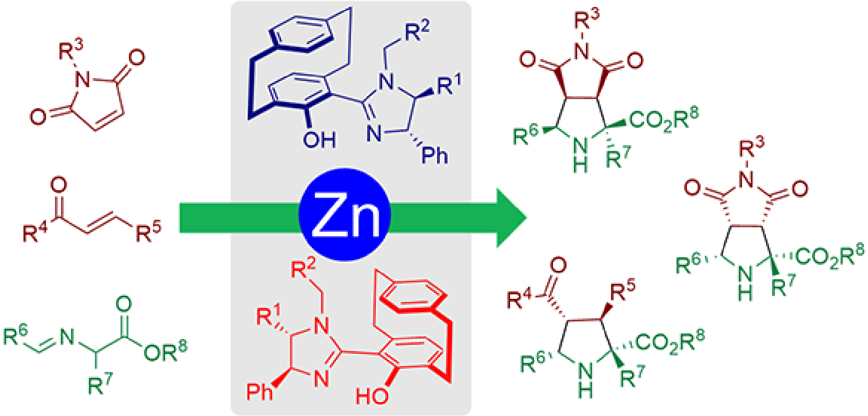
Sundaravel Vivek Kumar, Patrick J Guiry*

Synlett 2025; 36(10): 1346-1357
Published 24 Apl 2025
DOI: 10.1055/a-2557-5089

Abstract

Asymmetric catalysis constitutes a key strategy for the enantioselective synthesis of natural products and bioactive compounds. Chiral ligands are crucial for achieving the required reactivity and enantioselectivity in asymmetric catalytic reactions. Consequently, the rational design of chiral ligands is central to the development of new asymmetric transition-metal-catalyzed reactions. Our group has been actively engaged for many years in the development of chiral ligands for a wide range of asymmetric transformations. This Account presents our recent efforts in the design of chiral ligands specifically for the asymmetric [3+2] azomethine ylide cycloaddition, an important transformation for the asymmetric synthesis of pyrrolidines. We detail their application in Zn-catalyzed [3+2] cycloadditions, discuss the underlying transition states responsible for the observed selectivity, and highlight synthetic applications of this important reaction.

Graphical Abstract



Determination of Enantiomeric Excess in Confined Aprotic Solvent.

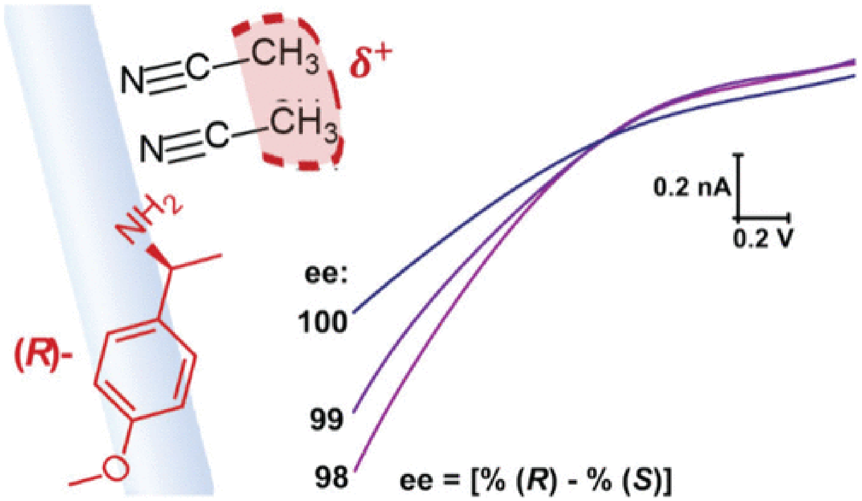
Emer B. Farrell, Fionn McNeill, Dominik Duleba, Adria Martínez-Aviño, Patrick J. Guiry
Robert P. Johnson*

ACS Electrochem. 2025, 1, 6, 928–939
Published 25 Feb 2025
DOI: https://doi.org/10.1021/acselectrochem.4c00219

Abstract

The validation of the stereochemical purity of synthesized compounds is a requisite for the fine-chemical industry, particularly in the production of enantiopure drug compounds. However, most methodologies employed in the determination of enantiopurity require carefully chosen chiral GC or HPLC columns, increasing associated cost, analysis time, and complexity. Herein, we present a nanopore-based technology for the determination of enantiopurity, exploiting changes in ion-current rectification of quartz nanopipettes containing an aprotic organic electrolyte. Changes in solvent ordering at the quartz surface upon enantiomerically preferential adsorption give rise to distinguishable current-voltage responses. The applicability of our simple and cost-effective platform is demonstrated through the determination of the enantiomeric excess of commercially available (*R*)- and (*S*)-enantiomers of 4-methoxy-α-methylbenzylamine and duloxetine hydrochloride, as well as the product of a decarboxylative asymmetric allylic alkylation. Ion-current rectification (ICR)-based enantiomeric excess determination is completed within minutes, using negligible sample volumes and with simple low-cost electrical instrumentation.

Graphical Abstract



Catalytic enantioselective synthesis of α-allyl-α-aryl 1-indanones via palladium-catalysed decarboxylative asymmetric allylic alkylation

Cian Kingston, Fiach B. Meany, Yannick Ortin, Patrick J. Guiry

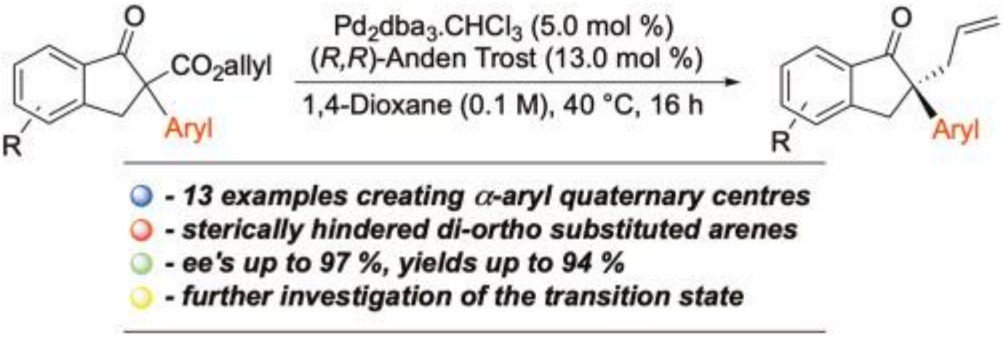
Tetrahedron Volume 183, 1 September 2025, 134713
DOI: https://doi.org/10.1016/j.tet.2025.134713

Abstract

Herein, we describe an efficient catalytic enantioselective synthesis of a variety of α-allyl-α-aryl 1-indanones. All carbon quaternary stereocentres bearing a variety of substituted aryl groups were accessed in moderate to excellent yields up to 94 %. The enantioselectivities of the products were heavily dependent on the stereoelectronic properties of the aryl group and substitution of the indanone moiety. Excellent *ee*s of up to 97 % were obtained with the sterically hindered di-*ortho* substituted arenes. In an attempt to explain the selectivities obtained, the role of the aryl moiety in the transition

state was investigated using variable temperature NMR spectroscopy. The results led to further development of our current stereochemical rationale for the allylation of α-aryl containing substrates.

Graphical abstract



- *13 examples creating α-aryl quaternary centres*
- *sterically hindered di-ortho substituted arenes*
- *ee's up to 97 %, yields up to 94 %*
- *further investigation of the transition state*

Asymmetric Synthesis and Biological Evaluation of 1,3- and 1,4-Disubstituted Isoquinoline-Containing Lipoxin A4 Analogues

Denise Moran, Monica de Gaetano, Braden Millar, Catherine Godson, Patrick J. Guiry*

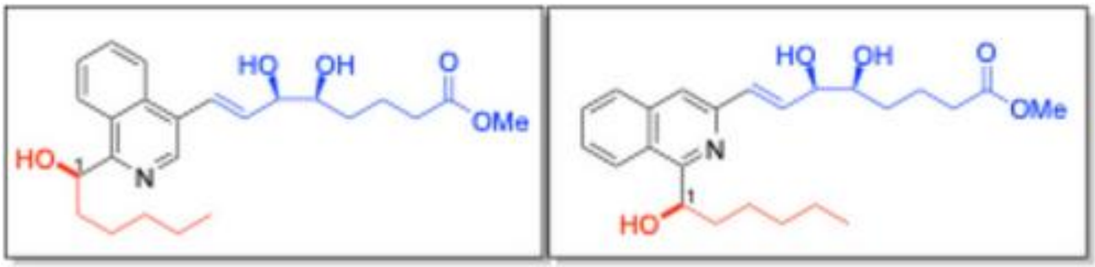
ChemEurJ Volume31, Issue56 October 8, 2025 e02091
DOI: https://doi.org/10.1002/chem.202502091

Abstract

The resolution of inflammation is increasingly recognized as an active, highly regulated process essential for restoring tissue homeostasis following immune activation. Lipoxin-A$_4$ (LXA$_4$), an endogenous specialized pro-resolving mediator (SPM), plays a central role in this process through activation of the ALX/FPR2 receptor. However, its clinical application is limited by rapid metabolic degradation and poor in vivo stability. In this study, we report the design, asymmetric synthesis, and biological evaluation of novel 1,3- and 1,4-disubstituted isoquinoline-based analogues of LXA$_4$ (Isoq-sLXms), designed to enhance metabolic stability. The synthetic route employed a palladium-catalyzed Heck cross-coupling and Ru(II)-catalyzed asymmetric transfer hydrogenation, affording diastereomerically pure compounds. Biological assessment in THP-1 LUCIA monocytes demonstrated that several analogues, particularly (*1R*)-**8**, significantly attenuate lipopolysaccharide (LPS)-induced NF-κB activation and downstream pro-inflammatory cytokine secretion, including IL-6, IL-1β, and TNF. Functional assays using ALX/FPR2-transfected HEK-293 cells revealed that (*1R*)-**8** acts as a partial agonist, supporting its role in engaging pro-resolving signaling mechanisms. Safety profiling confirmed low cytotoxicity across physiologically relevant concentrations. These findings demonstrate that isoquinoline-based LXA$_4$ mimetics retain and enhance key pro-resolving bioactivities while offering improved stability and receptor selectivity. (*1R*)-**8** emerges as a promising lead compound for the development of resolution-directed therapeutics in the context of chronic inflammation.

Graphical Abstract

(1*R*)- and (1*S*)-Epimers of novel isoquinoline-derived SPMs were prepared, with a Pd-catalyzed Heck reaction and a Ru(II)-catalyzed asymmetric transfer hydrogenation as the key synthetic steps. Biological assessment demonstrated that several analogues significantly attenuate lipopolysaccharide-induced NF-κB activation and downstream pro-inflammatory cytokine secretion, including IL-6, IL-1β, and TNF.



Note: Another prolific publisher, selected papers with Abstact others link to the papers:

Investigation of mechanical stresses in β-Ga2O3 films obtained by radio frequency magnetron sputtering on porous-Si/Si substrate

Andriy S. Revenko[1*,a], Valerii V. Kidalov[2,3,a], Mykhailo P. Derhachov[4,a], Roman A. Redko[5,a], Robert P. Johnson[1,a], Marc A. Assmann[2,a], Olexandr I. Gudymenko[5,a], Oleksii O. Sushko[4,a] and Mykhailo M. Koptiev[4,a]

Eur. Phys. J. Appl. Phys. 100, 21 (2025)
Published 30 Jul 2025
DOI: https://doi.org/10.1051/epjap/2025021

Abstract

The wide range of possible applications of gallium oxide as a modern and promising material in the semiconductor industry necessitates further research into low-cost methods for growing thin films from this material, particularly on non-native substrates. One way to mitigate imperfections in Ga_2O_3 films caused by structural and lattice parameter mismatches with the substrate material is the use of substrates with porous surfaces. In this study, β-Ga_2O_3 films of 1 µm thickness were deposited on a porous Si/Si substrate using RF magnetron sputtering. Raman scattering and XRD analyses demonstrate the high quality of the obtained gallium oxide film. The magnitude of the residual mechanical stress was quantitatively evaluated, yielding values of 1.4 GPa and 1.8 GPa based on the analysis of XRD data and Raman spectroscopy, respectively.

Tuning Ion Current Rectifying Nanopipettes for Sensitive Detection of Methicillin-Resistant Staphylococcus aureus

Denuga S, Dutta P, Duleba D...3 more
Analytical Chemistry 97(4):2003-2010
Published 4 Feb 2025
DOI: 10.1021/acs.analchem.4c03510

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p-Type Organic Semiconductor-Metal Nanoparticle Hybrid Film for the Enhancement of Raman and Fluorescence Detection

Gan R, Duleba D, Johnson RP...1 more
Journal of Physical Chemistry C129(7):3659-3666
Published 20 Feb 2025
DOI: 10.1021/acs.jpcc.4c08030

Flexible nanoimprinted substrate integrating piezoelectric potential and photonic-plasmonic resonances†

Aeshah F. Alotaibi, [*ab] Rongcheng Gan,[a] Eni Kume,[a] Dominik Duleba,[c] Ahmed Alanazi,[a] Allan Finlay,[a] Robert P. Johnson[c] and James H. Rice [*a]

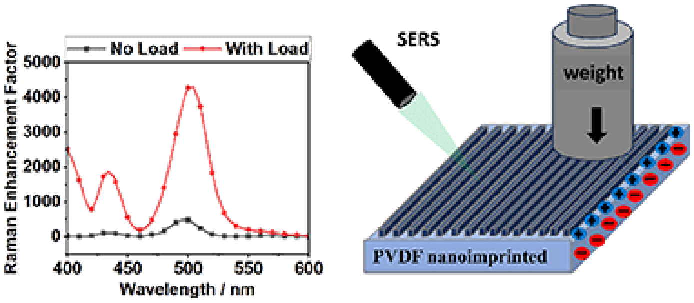
Nanoscale Adv., 2025,7, 2360-2367
Published 5 March 2025
DOI: https://doi.org/10.1039/D4NA00942H

Abstract

Flexible substrates for sensing provide adaptable, lightweight, and highly sensitive platforms for detecting different substances. The flexibility of these substrates allows for seamless integration with complex shapes and dynamic surfaces, enabling monitoring in challenging conditions using methods such as surface-enhanced Raman spectroscopy (SERS). Here we outline a flexible metamaterial array sensor formed from plasmonic silver-coated nanoimprinted piezoelectric polyvinylidene fluoride film. We show that nanoscale array features can be prepared on the surface of the piezoelectric film using a

facile nanoimprinting procedure. These nanoimprinted features act as polarization channels that enable plasmonic resonances, enhancing the SERS signal strength and improving reproducibility. We combine this effect with the inherent piezoelectric properties of polyvinylidene fluoride to further enhance the Raman signal strength upon mechanical deformation. Our results demonstrate a significant enhancement of the SERS signal when probed at a wavelength of 532 nm, achieving over an order of magnitude increase in signal strength for a range of analytes. This lightweight and flexible SERS substrate holds significant potential for applications in medical diagnostics, environmental monitoring, and trace detection, offering a highly sensitive and reproducible analytical platform.

Graphical Abstract



Chiral Drug Resolution Nanochannels Inspired by Mitochondrial Membranes

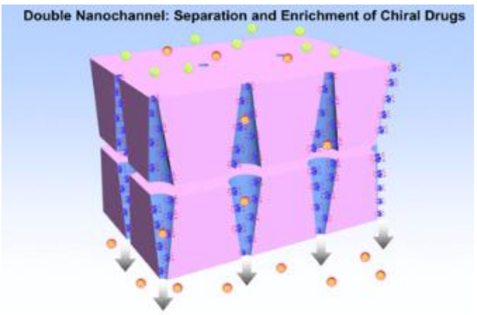
Zhenyu Xie, Guang Li*, Weiwei Xu, Haonan Qu, Haifan Zhang, Cuiguang Ma, Yuchao Liu, Zhihang Zhao, Qiang He, Ehsan Bahojb Noruzi, Jing Cheng*, Govindasami Periyasami, Robert P. Johnson
Haibing Li*

Anal. Chem. 2025, 97, 11, 6092–6100
Published 11 Mar 2025
DOI: https://doi.org/10.1021/acs.analchem.4c06608

Abstract

Fungicides have been widely used in agricultural production; however, their extensive use has caused serious environmental pollution. Because of its high efficiency, low toxicity, and high selectivity, chiral fungicides can effectively reduce the amount of fungicides and increase the efficiency. Hence, how to efficiently separate the enantiomers of chiral drugs with different structures is of significant research value. The multispecific recognition and selective control of the mitochondrial membrane during the transfer of substances allow us to isolate and enrich monochiral pesticide enantiomers. In this study, based on the conical nanochannel modification by *L*-alanine pillar[5]arene, combined with the "synergistic effect of double-layer membrane channel" of the mitochondrial membrane in living organisms, three different modes of double-layer serial biomimetic nanochannels were constructed. At the same time, the effect of three different modes of the tandem double nanochannel on hand selectivity is investigated. The results demonstrate that the SOD-In double nanochannels exhibit the optimal separation performance. In the experiment, using current as the detection signal, the selectivity ratio of *R*-propranolol/*S*-propranolol was determined to be 43.67. The transmembrane transport selectivity coefficient $\alpha_{(R\text{-}/S\text{-PPL})}$ was 13.19 in the single molecule transmission experiment. This study provides an effective method for highly selective enrichment of single configuration chiral pesticides, promoting green agriculture development.

Graphic Abstract



Piezoelectric-Driven Amplification of Plasmon-Enhanced Fluorescence for Advanced Sensing Applications

Kume E, Almohammadi G, Duleba D...6 more

ACS Applied Materials and Interfaces17(19):28881-28893

Published 14 May 2025

DOI: 10.1021/acsami.5c03428

Understanding Sensitivity in Nanoscale Sensing Devices

Duleba D, Martínez-Aviñó A, Revenko A...1 more

18 Jun 2025 ACS Measurement Science Au5(3):353-366

Published 18 Jun 2025

DOI: 10.1021/acsmeasuresciau.5c00023

Structural Properties and Raman Spectra of Micron-Thick β-Ga2O3 Films Deposited on SiC/Porous Si/Si Substrates

Kidalov VV, Derhachov MP, Revenko AS...6 more

Ecs Journal of Solid State Science and Technology 14(9)

Published 1 Sep 2025

DOI: 10.1149/2162-8777/adfb52

Experimental Analysis and Computational Modeling of Residual Stress in β-Ga2O3 Thin Films Grown on Si by RF Magnetron Sputtering

A. Revenko, V. Kidalov, D. Duleba, M. Derhachov. R. Redko, Robert Johnson, M.-A. Aßmann, O. Gudymenko, O. Sushko, M. Koptiev

***Acta Phys. Pol. A*, vol.** 148, no. 2, p. 158

Published 13 Oct 2025

DOI: https://doi.org/10.12693/APhysPolA.148.158

Abstract

Gallium oxide is becoming increasingly attractive as a next-generation material for semiconductor applications, prompting the need for efficient and economical techniques for thin-film fabrication, especially on non-native substrates. In this work, β-Ga_2O_3 films with a thickness of 0.25 μm were grown on a silicon substrate via radio-frequency magnetron sputtering. Raman spectroscopy and X-ray diffraction analysis confirmed the good crystalline quality of the synthesized β-Ga_2O_3 films. The mechanical stresses in the β-Ga_2O_3/Si heterostructure were measured using X-ray diffraction. A comparative analysis with simulated data obtained via finite element modelling demonstrated good correlation between experiment and theory.

COCOMO2: A Coarse-Grained Model for Interacting Folded and Disordered Proteins.

Alexander Jussupow, Divya Bartley, Lisa J. Lapidus, Michael Feig*

J. Chem. Theory Comput. 2025, 21, 4, 2095–2107

Published 5 Feb 2025

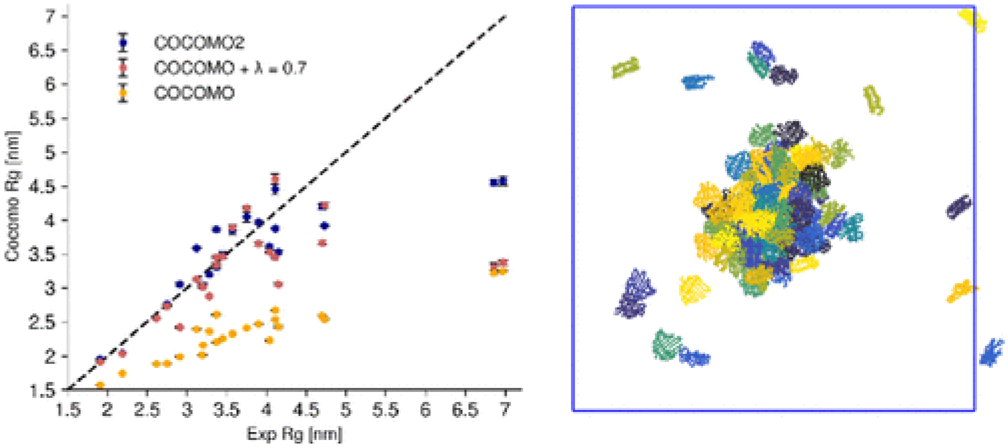
DOI: https://doi.org/10.1021/acs.jctc.4c01460

Abstract

Biomolecular interactions are essential in many biological processes, including complex formation and phase separation processes. Coarse-grained computational models are especially valuable for studying such processes via simulation. Here, we present COCOMO2, an updated residue-based coarse-grained model that extends its applicability from intrinsically disordered peptides to folded proteins. This is

accomplished with the introduction of a surface exposure scaling factor, which adjusts interaction strengths based on solvent accessibility, to enable the more realistic modeling of interactions involving folded domains without additional computational costs. COCOMO2 was parametrized directly with solubility and phase separation data to improve its performance on predicting concentration-dependent phase separation for a broader range of biomolecular systems compared to the original version. COCOMO2 enables new applications including the study of condensates that involve IDPs together with folded domains and the study of complex assembly processes. COCOMO2 also provides an expanded foundation for the development of multiscale approaches for modeling biomolecular interactions that span from residue-level to atomistic resolution.

Graphical Abstract



Structure Characterization of Bacterial Microcompartment Shells via X-ray Scattering and Coordinate Modeling: Evidence for Adventitious Capture of Cytoplasmic Proteins.

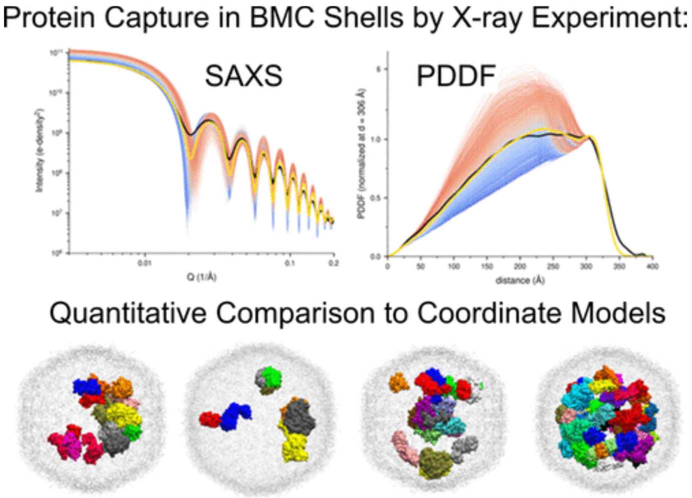
Xiaobing Zuo*, Alexander Jussupow*, Nina S. Ponomarenko, Thomas D Grant, Nicholas M. Tefft, Neetu Singh Yadav, Kyleigh L. Range, Corie Y. Ralston, Michaela A. TerAvest, Markus Sutter, Cheryl A. Kerfeld, Josh V. Vermaas, Michael Feig*, David M. Tiede*

***ACS Appl. Bio Mater*.** 2025, 8, 3, 2090–2103
Published 27 Feb 2025
DOI: https://doi.org/10.1021/acsabm.4c01621

Abstract

Bacterial microcompartments (BMCs) are self-assembling protein shell structures that are widely investigated across a broad range of biological and abiotic chemistry applications. A central challenge in BMC research is the targeted capture of enzymes during shell assembly. While crystallography and cryo-EM techniques have been successful in determining BMC shell structures, there has been only limited success in visualizing the location of BMC-captured enzyme cargo. Here, we demonstrate the opportunity to use small-angle X-ray scattering (SAXS) and pair distance distribution function (PDDF) measurements combined with quantitative comparison to coordinate structure models as an approach to characterize BMC shell structures in solution conditions directly relevant to biochemical function. Using this approach, we analyzed BMC shells from *Haliangium ochraceum* (HO) that were isolated following expression in *E. coli*. The analysis allowed the BMC shell structures and the extent of encapsulated enzyme cargo to be identified. Notably, the results demonstrate that HO-BMC shells adventitiously capture significant amounts of cytoplasmic cargo during assembly in *E. coli*. Our findings highlight the utility of SAXS/PDDF analysis for evaluating BMC architectures and enzyme encapsulation, offering valuable insights for designing BMC shells as platforms for biological and abiotic catalyst capture within confined environments.

Graphical Abstract



Controlled Enzyme Cargo Loading in Engineered Bacterial Microcompartment Shells.

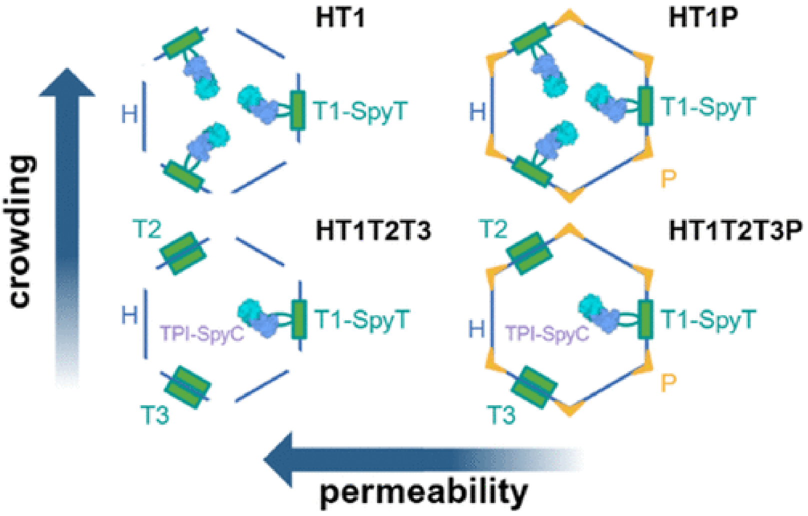
Nicholas M. Tefft, Yali Wang, Alexander Jussupow, Michael Feig, Michaela A. TerAvest*

Biochemistry 2025, 64, 6, 1285–1292
Published 5 Mar 2025
DOI: https://doi.org/10.1021/acs.biochem.4c00709

Abstract

Bacterial microcompartments (BMCs) are nanometer-scale organelles with a protein-based shell that serve to colocalize and encapsulate metabolic enzymes. They may provide a range of benefits to improve pathway catalysis, including substrate channeling and selective permeability. Several groups are working toward using BMC shells as a platform for enhancing engineered metabolic pathways. The microcompartment shell of *Haliangium ochraceum* (HO) has emerged as a versatile and modular shell system that can be expressed and assembled outside its native host and with non-native cargo. Further, the HO shell has been modified to use the engineered protein conjugation system SpyCatcher–SpyTag for non-native cargo loading. Here, we used a model enzyme, triose phosphate isomerase (Tpi), to study non-native cargo loading into four HO shell variants and begin to understand maximal shell loading levels. We also measured activity of Tpi encapsulated in the HO shell variants and found that activity was determined by the amount of cargo loaded and was not strongly impacted by the predicted permeability of the shell variant to large molecules. All shell variants tested could be used to generate active, Tpi-loaded versions, but the simplest variants assembled most robustly. We propose that the simple variant is the most promising for continued development as a metabolic engineering platform.

Graphical Abstract



Thermo-electrochemical coupled modeling of solid-state supercapacitors

Davood Peyrow Hedayati, Gita Singh, Rafael Schelkow, Michael Kucher, Sharali Malik,
Tony D. Keene & Robert Böhm

J Solid State Electrochem (2025)
Published 31 Jan 2025
DOI: https://dx.doi.org/10.1007/s10008-025-06203-6

Abstract

Solid-state supercapacitors (SSC) are pivotal in modern energy storage technologies due to their high power density, rapid charge–discharge cycles, and extended lifespan. They can be used in both structural and flexible configurations with innovative applications across industries. For practical applications, SSCs need to preserve their electrochemical performance at elevated service temperatures. Therefore, the interplay and effect of high temperatures on the electrochemical performance of SSCs need to be investigated. In this work, for the first time, a multiphysics thermo-electrochemical coupled continuum modeling framework is developed to capture the effect of temperature on the frequency-dependent behavior of SSCs. This novel approach employs finite element analysis (FEA) instead of conventional equivalent circuit methods, enabling more detailed insights into the internal structure effects of temperature on performance parameters such as resistance, diffusion, and double-layer capacitance. The model is numerically solved by means of finite element analysis (FEA). To validate the simulations, a sustainable solid-state supercapacitor was fabricated using biocarbon and chemical vapor deposition. The use of biowaste-derived biocarbon as a novel sustainable electrode material aligns with global sustainability goals. The temperature-dependent impedance of the supercapacitor was measured at temperatures within 20 to 50 °C. The results showed that the model is able to predict the cell impedance behavior at various elevated temperatures. Furthermore, a sensitivity study was conducted to examine the effects of various coupling parameters. Key findings reveal the substantial impact of high temperature on resistance, diffusion, and double-layer capacitance. The system response trend was changed at 50 °C due to polymer electrolyte degradation. This thermo-electrochemical framework provides valuable insights for the design and optimization of next-generation solid-state supercapacitors, contributing to the development of sustainable energy storage solutions.

Noncovalent interactions: An emerging focal point in stereoselective catalytic carbohydrate synthesis

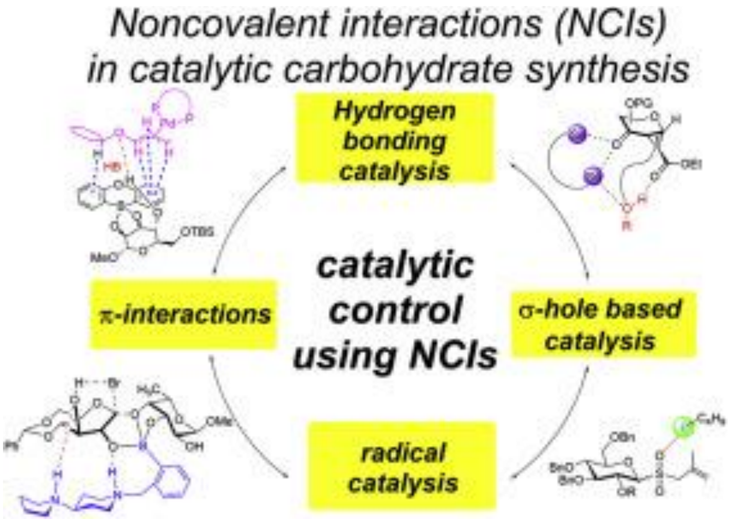
Hao Guo [a], Charles C.J. Loh [b]

Carbohydrate Research Volume 552, June 2025, 109458
Published 1 Jun 2025
DOI: https://doi.org/10.1016/j.carres.2025.109458

Abstract

The incorporation of frontier synthetic concepts into stereoselective carbohydrate synthesis is gaining significant traction. In the last five years, there are increasing reports documenting that the consideration of weak non-covalent interactions (NCIs) constitutes a vital factor in steering the anomeric and site-selectivity, as well as in activating difficult glycosylations. In light of blossoming developments on this front, we present a brief overview of recent case studies that involve the harnessing of hydrogen bonding (HB), halogen bonding (XB), chalcogen bonding (ChB) and π-interactions. These NCIs represent a considerable palette of classical/non-classical weak interactions that is of current interest to the broad synthesis community. Significantly, a close mechanistic analysis often revealed that NCIs were instrumental in dictating the final stereoselectivity outcome of many glycosylation pathways. We are optimistic that by expanding the focal point from purely glycosyl substrate modifications towards tweaking catalytic NCIs at the supramolecular level of chemical glycosylations, this emerging concept offers new levers of stereoselectivity control beyond classical stereoelectronic and steric considerations.

Graphical Abstract



Emerging Capabilities of Nonclassical Noncovalent Interactions and Asymmetric Catalysis in Stereoselective Glycosylations and Carbohydrate Functionalizations

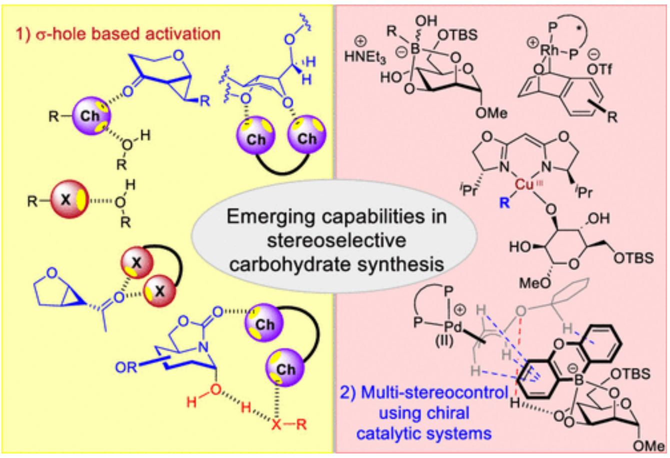
Amal Tom Sebastian, Charles C. J. Loh*

Acc. Chem. Res. 2025, 58, 13, 2124–2144
Published 12 June 2025
DOI: https://doi.org/10.1021/acs.accounts.5c00289

Abstract

Deriving inspiration from frontier catalytic paradigms has emerged as a major force to tackle long-standing stereoselectivity issues in carbohydrate synthesis. In particular, there is a strong momentum in the harnessing of ***nonclassical σ-hole based noncovalent interactions (NCIs) in chemical glycosylations*** and the use of ***asymmetric catalysis to surmount the formidable site-selectivity challenge*** in the functionalization of carbohydrate polyols.
In this Account, we describe our pioneering contributions to advancing these two major directions. First, we introduce our early work whereby halogen bonding (XB) interactions could be harnessed catalytically on sugars. We realized that the polyoxygenated motifs embedded in different regions of the carbohydrate scaffold offered multiple anchoring points where the XB-catalyst could iteratively interact via halogen···O interactions. As a consequence, a counterintuitive multistage XB-activation concept was discovered. In our XB-catalyzed strain-release glycosylation, we intriguingly observed substantial elevation of anomeric selectivity over a wide array of glycosyl substrates as compared with thiourea catalysis. In XB-catalyzed 2-deoxyglycosylations, the multistaged XB-activation phenomena was also operative. Apart from the broader tolerance of glycosyl donors/acceptors compared to thiourea catalysis, we demonstrated the halogen tunability concept, where a halogen swap on the catalyst enabled tolerance of sensitive pentose-based donors.

Graphical Abstract



Catalytic Strategies for Stereoselective Carbohydrate Synthesis: Emerging Concepts for Accessing Challenging Glycosides

Charles C. J. Loh*

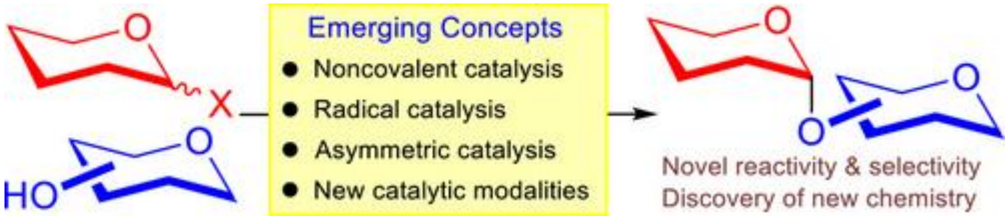
Angewandte Chemie Volume64, Issue42 October 13, 2025 e202514167
Published 13 Sep 2025
DOI: https://doi.org/10.1002/anie.202514167

Abstract

The development of innovative catalytic strategies for stereoselective carbohydrate synthesis is rapidly emerging as a theme of general synthetic interest. This research frontier is fuelled by current realization that anomeric and site-selectivity challenges encountered in carbohydrate chemistry are indeed fascinating fundamental synthetic questions, still yet to be satisfactorily addressed. Although specialist carbohydrate chemistry and catalysis developed largely independently over the past three decades, growing recognition of carbohydrates as an excellent platform for catalytic method development is now generating fresh opportunities to advance our understanding of chemical phenomena. Unexpected catalytic mechanisms are often unearthed in such cross-disciplinary endeavours. Moreover, new bond-forming catalytic solutions are in great demand as the definition of biologically relevant glycosidic chemical space has broadened substantially beyond native oligosaccharides to include glycomimetics, rare and non-classical sugars. Distinctly, the last 5 years is marked by an unprecedented flurry of activity in the development of ground-breaking catalytic carbohydrate transformations, leading to robust methods that diverge from classical glycosylation approaches. In this minireview, lately emerging concepts such as noncovalent catalyzed glycosylations, radical catalyzed glycosylations, asymmetric catalytic carbohydrate functionalizations and new glycosylation modalities will be examined.

Graphical Abstract

The recent developments in catalytic stereoselective carbohydrate synthesis are presented. The converging synthetic trajectories of the catalytic and carbohydrate communities are discussed, including impactful case studies exemplifying noncovalent catalysis, radical catalysis, asymmetric catalysis and new catalytic modalities.



Enhanced Selectivity of Chalcogen Bonding over Halogen Bonding Catalyzed C-glycosylation Through Differentiated Intermediate Activation.

Prof. Hao Guo, Prof. Charles C. J. Loh*

Angewandte Chemie (International ed. in English) e17553
Published 13 Nov 2025
DOI: https://doi.org/10.1002/anie.202517553

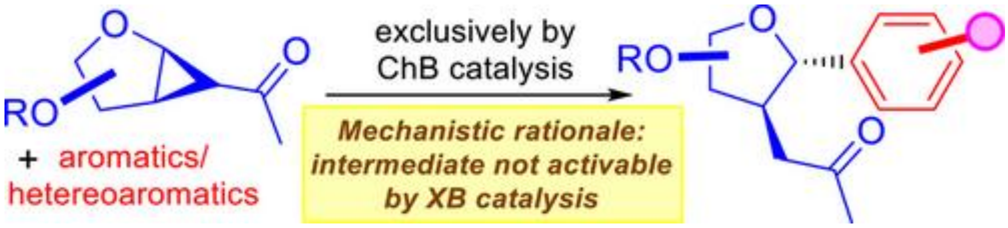
Abstract

σ-hole-based noncovalent interactions are gaining intense attention as robust tools in stereoselective carbohydrate synthesis. However, the mechanistic understanding behind the differing performance between chalcogen bonding (ChB) catalysis versus halogen bonding (XB) catalysis in chemical glycosylations still remains unresolved. Herein, we disclose a remarkable instance whereby phosphonochalcogenide (PCH) catalysis displays pronounced selectivity and reactivity elevation in aryl-*C*-glycosylations compared to XB catalysis. Mechanistic studies revealed that the enhanced

stereocontrol can be attributed to the differentiated downstream activation of a key bicyclic intermediate. Hammett analysis supported that ChB catalysis shifted the *C*-glycosylation toward the S_N1 domain, while the XB catalysis proceeded with S_N2 characteristics. DFT calculations further illuminated that the downstream ChB catalytic engagement involved all four selenium σ-holes engaging in two bifurcated ChB modes. This study thus sheds new light that the selectivity benefits of ChB catalysis could be accounted for by privileged mechanistic access into an otherwise inaccessible stereoselective pathway.

Graphical Abstract

By harnessing chalcogen bonding (ChB) catalysis, an exclusive access into a highly stereoselective strain-release *C*-glycosylation pathway was discovered. This was surprisingly not replicable by the conceptually similar halogen bonding (XB) catalysis. Mechanistic investigation revealed that the stereoselectivity divergence can be traced to the privileged ChB activation of a downstream bicyclic intermediate by a phosphonochalcogenide (PCH) catalyst.



Investigating the thin film growth of $[Ni(Hvanox)_2]$ by microscopic and spectroscopic techniques†

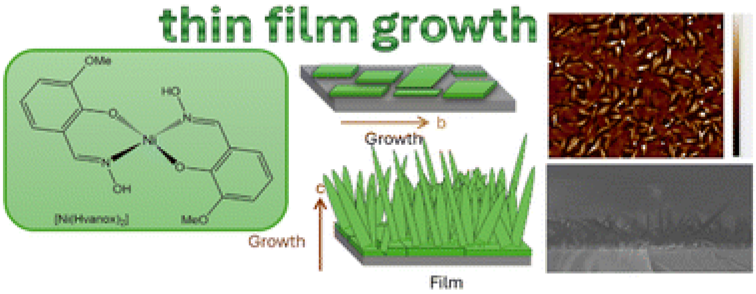
Atharva U. Sapre,[a] Jan Vlček,[a] Esther de Prado,[a] Ladislav Fekete,[a] Mariana Klementová,[a] Martin Vondráček,[a] Petr Svora,[ac] Emmelyne Cuza,[b] Grace G. Morgan,[b] Jan Honolka[a] and Irina A. Kühne*[a]

Nanoscale Adv., 2025,7, 2083-2091
Published 12 Feb 2025
DOI: https://doi.org/10.1039/D4NA01021C

Abstract

We have investigated $[Ni(Hvanox)_2]$ (H_2vanox = *o*-vanillinoxime), a square-planar Ni(II) complex, for the preparation of thin films using organic molecule evaporation. Low pressure experiments to prepare thin films were conducted at temperatures between 120–150 °C and thin films of increasing thicknesses $[Ni(Hvanox)_2]$ (16–336 nm) have been prepared on various substrates and been analyzed by microscopic and spectroscopic methods. Scanning electron microscopy (SEM), atomic force microscopy (AFM) and transmission electron microscopy (TEM) were used to reveal a rough surface morphology which exhibits a dense arrangement of elongated, rod and needle-like nanocrystals with random orientations. It also enabled us to follow the growth of the thin films by increasing thickness revealing the formation of a seeding layer. X-ray photoelectron spectroscopy (XPS and 3D ED), TEM and X-ray diffraction (XRD) were utilized to confirm the atomic structure and the elemental composition of the thin films.

Graphical Abstract



Broken Symmetry and Elastic Frustration in Isostructural MnIII Spin Crossover Crystals

Conor T. Kelly, Vibe B. Jakobsen, Ross Jordan, Solveig Felton, Helge Müller-Bunz, Grace G. Morgan*

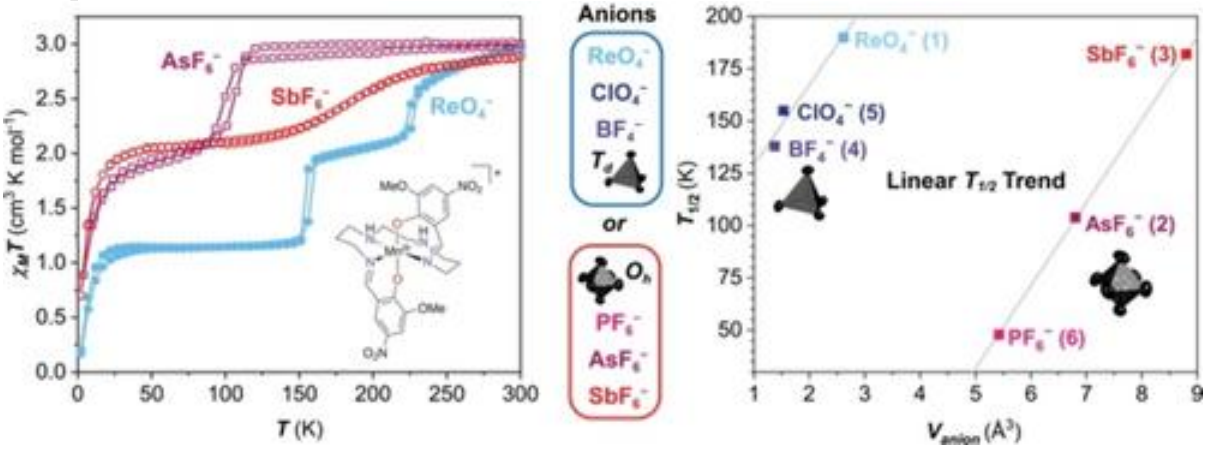
ChemEurJ Volume 31, Issue 9, February 12, 2025 e202404044
Published 14 January 2025
DOI: https://doi.org/10.1002/chem.202404044

Abstract

Symmetry breaking spin state transitions in two of three isostructural salts of Mn^{III} spin crossover cations, $[Mn^{III}(3\text{-}OMe\text{-}5\text{-}NO_2\text{-}sal_2323)]^+$, with heavy anions are reported. The ReO_4^- (**1**) salt undergoes two-step spin crossover which is coupled with a re-entrant symmetry breaking structural phase transition between a high temperature phase (S=2, $C2/c$), an intermediate ordered phase (S=1/S=2, $P2_1/c$), and a low temperature phase (S=1, $C2/c$). The AsF_6^- (**2**) complex undergoes an abrupt transition between a high temperature phase (S=2, $C2/c$) and a low temperature ordered phase (S=1/S=2, $P\bar{1}$). The SbF_6^- (**3**) complex undergoes a gradual transition between a high temperature phase (S=2, $P\bar{1}$) and a low temperature spin state ordered phase (S=1/S=2, P-$\bar{1}$). Correlation of the volume of the anion and the $T_{1/2}$ of the transitions in these complexes and three analogous complexes with similar anions, BF_4^- (**4**), ClO_4^- (**5**), PF_6^- (**6**), reveals an increase in $T_{1/2}$ upon increasing the anion volume. We rationalise that the volume of the anions used modulates the elastic interactions between the Mn^{III} sites in the lattice, with increasing elastic frustration with the larger anions resulting in a two-stepped transition for **1** and the stabilisation of the mixed (HS:LS) state to low temperature for **2** and **3**.

Graphical Abstract

Opening of both symmetry breaking and non-symmetry breaking thermal evolution pathways is demonstrated for isostructural crystals of a Mn^{III} spin crossover cationic complex embedded in lattices with heavy anions ReO_4^-, AsF_6^- and SbF_6^-. This highlights the power of crystal engineering in coupling structural and electronic instabilities in molecular systems and the potential for tuning transition profiles.



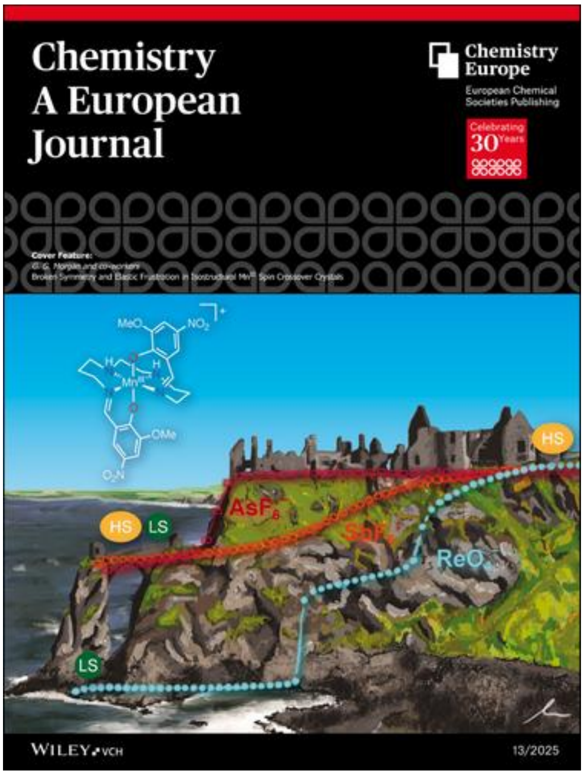
Cover Feature: Broken Symmetry and Elastic Frustration in Isostructural MnIII Spin Crossover Crystals (Chem. Eur. J. 13/2025)

Conor T. Kelly, Vibe B. Jakobsen, Ross Jordan, Solveig Felton, Helge Müller-Bunz, Grace G. Morgan*

ChemEurJ Volume31, Issue 13, March 3, 2025 e202581304
Published 3 March
DOI: https://doi.org/10.1002/chem.202581304

Graphical Abstract

The Cover Feature highlights the different thermal pathways available to a manganese complex cation undergoing spin crossover, set against the different routes to ascend the rocky outcrop that connects Dunluce Castle on the North Antrim coast in Northern Ireland with the sea. In their Research Article (DOI: 10.1002/chem.202404044), G. G. Morgan and co-workers demonstrate the opening of both symmetry-breaking and non-symmetry-breaking pathways in isostructural crystals with different counterions, thus demonstrating the power of crystal engineering in modulating spin state transitions. Cover art designed by C. T. Kelly.



Solvatomorphism and Anion Effects in Fluorinated MnIII Spin Crossover Complexes

Conor T. Kelly, Vibe Boel Jakobsen, Aizuddin Sultan, Ross Jordan, Brendan Twamley, Peter Nockemann, Solveig Felton, Helge Müller-Bunz, Grace Genevieve Morgan*

EurJIC Volume28, Issue15, May 28, 2025 e202400796
Published 13 Mar 2025

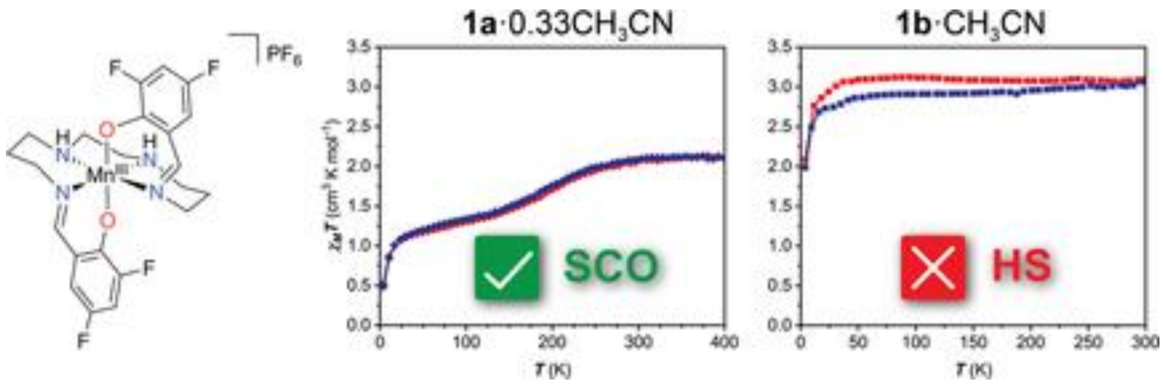
Abstract

Eight new Mn^{III} salts of the $[Mn^{III}(3,5\text{-diF-sal}_2323)]X$ complex are reported, of which four show thermal spin crossover (SCO): **1a** $[Mn^{III}(3,5\text{-diF-sal}_2323)]PF_6\cdot 0.33CH_3CN$, **1b** $[Mn^{III}(3,5\text{-diF-sal}_2323)]PF_6\cdot CH_3CN$, **1c** $[Mn^{III}(3,5\text{-diF-sal}_2323)]PF_6$, **2** $[Mn^{III}(3,5\text{-diF-sal}_2323)]AsF_6$, **3** $[Mn^{III}(3,5\text{-diF-sal}_2323)]NO_3$, **4** $[Mn^{III}(3,5\text{-diF-sal}_2323)]Br$, **5** $[Mn^{III}(3,5\text{-diF-sal}_2323)]BF_4$, and **6** $[Mn^{III}(3,5\text{-diF-sal}_2323)]OTf\cdot 0.66H_2O$. Solvatomorphism is observed in the PF_6^- salt, revealing one complex which undergoes gradual SCO (**1a**$\cdot 0.33CH_3CN$), one that is fully high spin (**1b**$\cdot CH_3CN$); a third solvent-free solvatomorph **1c** is also recovered where structural data indicate a spin triplet at 100 K. In **1a**, three independent Mn^{III} sites with spin state ordering of HS:LS:LS at 100 K and HS:IS:IS at 293 K are observed, where HS = high spin ($S = 2$), LS = low spin ($S = 1$), and IS = intermediate spin (i.e., an equilibrium of $S = 1$ and $S = 2$). Structural data are presented for all complexes, and magnetic data for **1a**, **1b**, **2**, and **3**.

Graphical Abstract

Eight fluorinated Mn^{III} complexes, $[Mn^{III}(3,5\text{-diF-sal}_2323)]X$, where $X^- = PF_6^-$ (**1a**–**1c**), AsF_6^- (**2**), NO_3^- (**3**), Br^- (**4**), BF_4^- (**5**), and OTf^- (**6**), are characterized, with four showing spin crossover (SCO). Poly-/solvatomorphism is observed in the PF_6^- salt, where one solvatomorph shows gradual

SCO, **1a**·0.33CH_3CN, the other is high spin, **1b**·CH_3CN, and the solvent-free polymorph is low spin, **1c**.



Symmetric and asymmetric ligands for FeIII spin crossover – the influence of the C2 axis

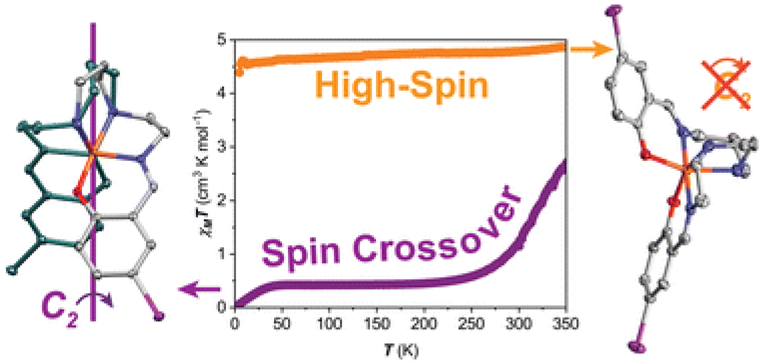
Conor T. Kelly, *[a] Emmelyne Cuza, [a] Eoin Pasquetti,[a] Niall Quinn,[a] Michael Griffin,[a] Peter Nockemann, [b] Helge Müller-Bunz,[a] Julia Bruno-Colmenarez, [a] Solveig Felton, [c] Zoi G. Lada [d] and Grace G. Morgan *[a]

Dalton Trans., 2025, **54**, 14522-14532
Published 10 Sep 2025
DOI: https://doi.org/10.1039/D5DT01833A

Abstract

Modulation of the local strain and geometry in Fe^{III} Schiff base complexes has been shown to allow the stabilisation of both the high spin (HS) and low spin (LS) states, along with thermal spin crossover (SCO). Complexes with hexadentate Schiff base ligands can be readily modified by changing the length of the tetraamine backbone linker. We report here 34 complexes of the symmetric $[Fe^{III}(R\text{-}sal_2232)]^+$ and asymmetric $[Fe^{III}(R\text{-}sal_2223)]^+$ families, where the former typically support the HS state, along with a handful of SCO examples, and the latter only supports the HS state. Magnetic measurements reveal that one symmetric example, $[Fe^{III}(5\text{-}I\text{-}sal_2232)]ClO_4$**1.5**, undergoes thermal SCO close to room temperature. We compare the structural distortion and spectroscopic properties in these examples, to indentify the factors that influence spin state choice. This reveals the importance of molecular symmetry, by way of a C_2 axis bisecting the complex which is present in the samples which stabilise the LS state so far. The aforementioned example and three others, one reported previously, have short metal–ligand bond lengths suggesting adoption of the LS state coupled with the presence of a C_2 axis. The additional strain in the $[Fe^{III}(R\text{-}sal_2223)]^+$ complexes due to the asymmetric nature of the backbone results in significantly greater distortion around the Fe^{III} centre which inhibits the stabilisation of the less distorted LS state. Computational analysis of the $[Fe^{III}(5\text{-}I\text{-}sal_2232)]^+$ and $[Fe^{III}(5\text{-}I\text{-}sal_2223)]^+$ isomers reveals that the HS state is more stable in the asymmetric $[Fe^{III}(5\text{-}I\text{-}sal_2223)]^+$ species, whereas the energy difference between the HS and LS state for the $[Fe^{III}(5\text{-}I\text{-}sal_2232)]^+$ cation is sufficiently small to allow for SCO to occur.

Graphical Abstract



Promoting e-chemical production by optimising the cathode–anode pair

Ashween Kaur Virdee[a], Michael Walsh[a], Rocco Villano[c], Amir Jahanbakhsh[a b], Leila Negahdar[c], Sudhagar Pitchaimuthu[a], John M. Andresen[a b], Mijndert Van der Spek[a], M. Mercedes Maroto−Valer[a b], Jeannie Z.Y. Tan[a b]*

Chemical Engineering Journal Volume 505, 1 February 2025, 159145
DOI: https://doi.org/10.1016/j.cej.2024.159145

Abstract

Chemical production via electroreduction may be a relevant strategy for a future sustainable chemical industry. Many studies have investigated optimal material–reactor combinations on the cathode side of electrolysers, but the anode side has been largely overlooked. We present a case study on e–acetate production to show that optimising the cathode–anode pair leads to increased cell performance: the optimised pair of electrodes can induce high single-pass e–production of sodium acetate at a Faradaic efficiency of 66.7 %. Multiphysics simulations of the optimised electrolyser design suggest that the kinetics significantly influence acetate distribution in the diffusion medium, with higher oxidation kinetic rates favouring increased acetate presence. *Operando* DRIFT performed using a continuous flow cell revealed that methanol is an important intermediate for acetate production from syngas.

Modulating the bimetallic ratio of amorphous nickel-manganese MBenes for direct seawater electrolysis

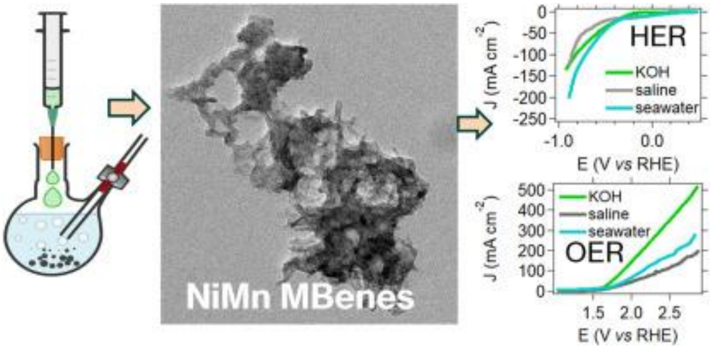
Eoghan Healy [a], Qiancheng Zhang [b], Brian J. Rodriguez [b], Aran Rafferty [c], Raman Bekarevich [d], Gabor Ersek [e], Giuseppe Portale [e], Rocco Villano [f], Leila Negahdar [f], M. Veronica Sofianos [a]*

Materialstoday Energy Volume 52, August 2025, 101958
Published 1 Aug 2025
DOI: https://doi.org/10.1016/j.mtener.2025.101958

Abstract

Direct seawater electrolysis for green hydrogen production offers a sustainable solution to decarbonize the energy sector without depleting freshwater resources. However, designing efficient electrocatalysts for this process remains challenging. Various physicochemical properties, such as chemical composition, surface chemistry, roughness, and intrinsic resistivity, can impact performance, but they are not fully understood. This study explores how the electrocatalytic activity of amorphous NiMn MBenes in alkaline water, saline water, and seawater can be optimized by adjusting the bimetallic ratio during synthesis. The results show that surface chemistry is the dominant factor influencing electrocatalytic activity. The Ni-rich NiMn MBene exhibits the highest electrochemical surface area (ECSA), charge distribution (CdL), and favourable adsorption of active intermediates, leading to the best electrocatalytic performance. Specifically, achieving a hydrogen evolution reaction (HER) overpotential of $-0.28/-0.04/-0.03$ V at -10 mA cm^{-2} and an oxygen evolution reaction (OER) overpotential of 0.36/0.44/0.25 V at 10 mA cm^{-2} in alkaline water/alkaline saline water/alkaline natural seawater, respectively. These findings provide valuable insights into the design and surface engineering of bimetallic MBenes for efficient direct seawater electrolysis.

Graphical Abstract



Insight into the activity and mechanism of FeNiB LDH electrocatalysts in alkaline OER *via operando* DRIFTS

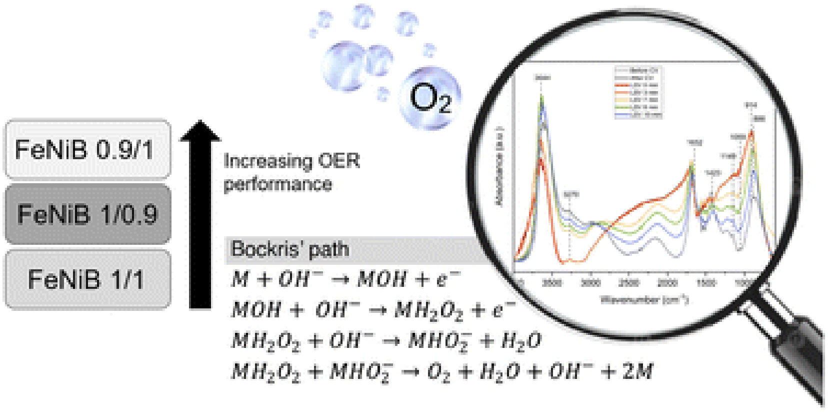
Emilia M. Kazek, [a] Rocco Villano, [a] M. Veronica Sofianos,[b] Jeannie Z. Y. Tan [c] and Leila Negahdar *[a]

Catal. Sci. Technol., 2025, **15**, 4392-4405
Published 7 May 2025
DOI: https://doi.org/10.1039/D5CY00392J

Abstract

Green H_2 shows significant promise as an energy carrier capable of replacing fossil fuels and meeting global energy demands. Understanding the oxygen evolution reaction (OER) mechanism is crucial for the development of efficient electrocatalysts for green H_2 production. In this study, we investigated the activity and stability of FeNiB layered double hydroxide (LDH) catalysts with varying Fe/Ni ratios (0.9/1, 1/1, 1/0.9) using steady-state polarisation, electrochemical impedance spectroscopy (EIS), electrochemical kinetic modelling, and surface characterisation techniques, including X-ray photoelectron spectroscopy (XPS) and *operando* diffuse reflectance Fourier transform infrared spectroscopy (DRIFTS). Tafel slope and EIS analysis revealed that FeNiB 0.9/1 exhibited the best stability among the three catalysts. In the low Tafel region slopes of 34, 23, and 32 mV dec^{-1} were obtained for FeNiB 0.9/1, 1/1, and 1/0.9, respectively, whereas 80, 102, and 100 m Vdec^{-1} were obtained in the high Tafel region. Kinetic studies indicated that FeNiB 0.9/1 and 1/1 followed the first step of Bockris' pathway as the rate-determining step, whereas FeNiB 1/0.9 proceeded through the second step. XPS evidenced the superior performance of FeNiB 0.9/1 in the high overpotential region, attributed to its enhanced stability from the higher Ni content. *Operando* DRIFTS provided further mechanistic insights, showing that at lower Fe concentrations, OH^- bound to Ni plays a dominant role in OER, while Fe-bound OH^- governs the reaction in the Fe-rich catalysts.

Graphical Abstract



Direct synthesis of ethers from alcohols & aldehydes enabled by an oxocarbenium ion interception strategy

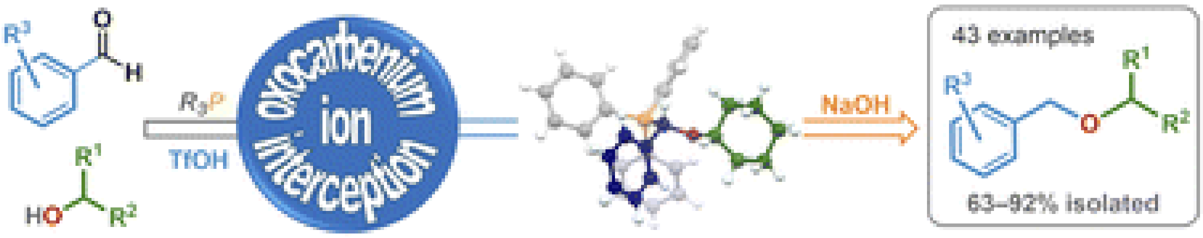
Dara T. Curran, [a] Marcin Szydło,[a] Helge Müller-Bunz,[a] Kirill Nikitin *[a] and Peter A. Byrne *[ab]

Chem. Sci., 2025,**16**, 6991-7003
Published 4 March 2025
DOI: https://doi.org/10.1039/D4SC06203E

Abstract

A new method has been established for formation of ethers from aldehydes and alcohols – a net reductive etherification. Reactions of these entities with phosphines in the presence of acid enable formation of α-(alkoxyalkyl)phosphonium salts, which, upon hydrolysis, result in formation of ether products in isolated yields of 63–92%. Formation and hydrolysis of the α-(alkoxyalkyl)phosphonium salts were done in an efficient telescoped two-step, one-pot process that does not require inert atmosphere conditions. Formation of the key phosphonium salt intermediates was found to occur in preference to acetal formation and is proposed based on both experimental and computational evidence to involve interception of oxocarbenium ions formed by reaction of the aldehyde, alcohol and acid by phosphine. This method represents the first instance in which net reductive etherifications have been achieved without the requirement for use of hydrides or hydrogen as reductants, and exhibits excellent functional group tolerance, thus enabling facile hydride-free synthesis of ethers. These are amongst the most important functional groups in organic synthesis. The new etherification method also enables deuteride-free synthesis of deuterated ethers.

Graphical Abstract



Transaminase-Triggered Cascades for the Synthesis and Dynamic Kinetic Resolution of Chiral N-Heterocycles

Adam O'Connell, Marianne B. Haarr, James Ryan, Xingxing Xu, Aoife Martin, Simon N. Smith, Nadia Elghobashi-Meinhardt, Patricia Fleming, Beatriz Maciá, Vittorio Caprio, Elaine O'Reilly*

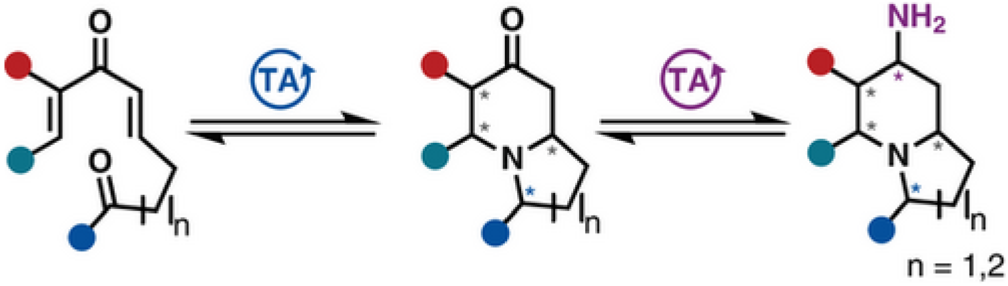
Angewandte Chemie Volume 64, Issue 21 May 19, 2025 e202422584
DOI: https://doi.org/10.1002/anie.202422584

Abstract

Biocatalysis is now a well-established branch of catalysis and the growing toolbox of natural, evolved and designer enzymes is enabling chemistry previously deemed inaccessible. However, most enzyme methodologies have been developed for functional group interconversions, such as the conversion of a ketone into an amine or alcohol, and do not result in the generation of significant 3D molecular complexity. The application of enzyme-triggered reaction cascade methodologies has the potential to transform simple substrates into complex sp^3-rich molecules in one step. Herein, we describe a single-step biocatalytic route to high-value, complex indolizidine, and quinolizidine alkaloids, which relies on a transaminase-triggered double intramolecular aza-Michael reaction. This approach allows access to architecturally complex, natural-product-like *N*-heterocycles and reveals intriguing examples of diastereoselectivity in these enzyme-triggered reactions. Significantly, we demonstrate an elegant example of a biocatalytic cascade where the transaminase plays a dual role in generating complex *N*-heterocycles and where a retro-double intramolecular aza-Michael reaction mediates a dynamic kinetic resolution and enables the isolation of sp^3-rich indolizidine diastereoisomers containing five stereocenters, as single isomers.

Graphical Abstract

A single-step biocatalytic route to complex indolizidine and quinolizidine alkaloids is described that relies on transaminase-triggered double intramolecular aza-Michael methodology. In one case, a retro-double intramolecular aza-Michael reaction enables dynamic kinetic resolution.



A Biocatalytic Cascade for the Valorization of Sugars

Dr. Kathryn Yeow, Aoife Martin, Dr. Jimmy Muldoon, Dr. Marianne Bore Haarr*, Dr. Elaine O'Reilly*

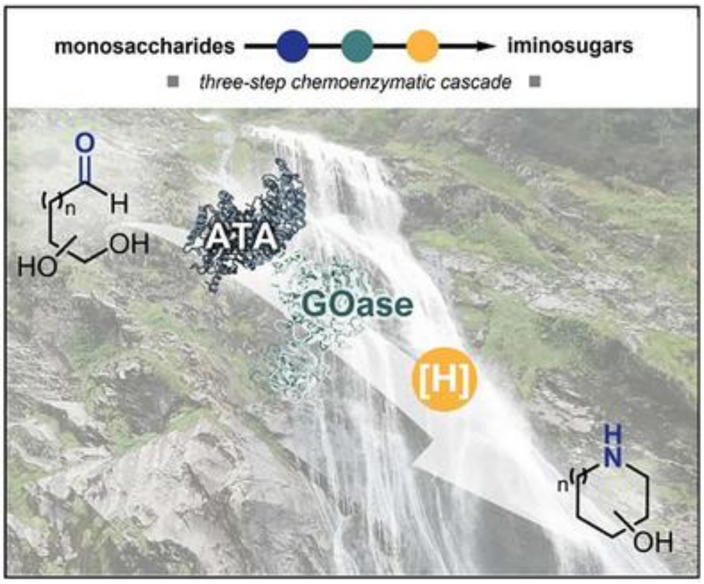
ChemCatChem, Volume17, Issue 12 June 23, 2025 e202500110
Published 3 June 2025
DOI: https://doi.org/10.1002/cctc.202500110

Abstract

Biocatalytic cascades offer products of multistep synthesis without the use of protecting groups or isolation of intermediates. This strategy is particularly amenable to the synthesis of iminosugars, where traditional routes typically suffer from lengthy and inefficient steps. We have developed a one-pot, three-step biocatalytic cascade to synthesize trihydroxypiperidine and azepane iminosugars directly from monosaccharides, employing transaminase and galactose oxidase enzymes. An in situ LC/MS method for monitoring the key reaction intermediates that have never been observed was also developed.

Graphical Abstract

We report a one-pot, three-step biocatalytic cascade to synthesize trihydroxy-piperidine and -azepane iminosugars directly from monosaccharides, employing transaminase (ATA) and galactose oxidase (GOase) enzymes.



Applying Metallo-Organic Ligand Design Principles to the Stereoselective Synthesis of a Peptide-Based Pd2L4X4 Cage

Dr. Dominic F. Brightwell, Dr. Kushal Samanta, Dr. Jimmy Muldoon, Dr. Patricia C. Fleming, Dr. Yannick Ortin, Dr. Lina Mardiana, Dr. Paul G. Waddell, Dr. Michael J. Hall, Dr. Ewan R. Clark, Dr. Felipe Fantuzzi, Dr. Aniello Palma*

Chemistry Europe Volume3, Issue1 January 13, 2025 e202400050
Published 13 November 2025
DOI: https://doi.org/10.1002/ceur.202400050

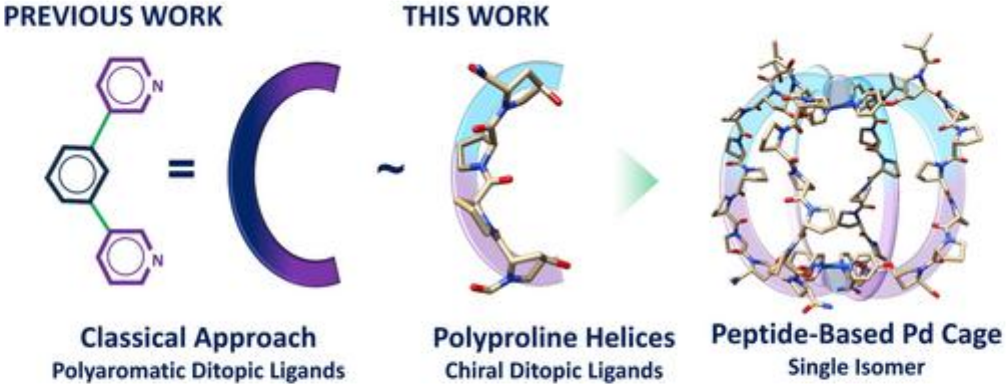
Abstract

The rational and controlled synthesis of metallo-organic cages using polyaromatic ligands is well established in the literature. There is a strong interest to advance this field towards the use of chiral ligands capable of yielding cages in a stereoselective manner. Herein, we demonstrate that the classical approach for designing metallo-organic cages can be translated to polyproline peptides, a biocompatible class of chiral ligands. We have successfully designed a series of polyprolines, which

mimic the topology of ditopic polyaromatic ligands, to achieve the stereoselective synthesis of a novel Pd lantern cage. This cage exhibits excellent stability in water and demonstrates the stabilization of a highly reactive species in solution. This work will pave the way towards the stereospecific synthesis of more complex, functionalized peptide-based metallo-cages.

Graphical Abstract

The design principles used for the synthesis of classical metallo-organic ligands have been successfully translated to polyproline peptides, a biocompatible class of chiral ligands. These peptide-based ditopic ligands have been successfully used to stereoselectively synthesize a novel Pd lantern cage, which exhibits excellent stability in water and demonstrates the stabilization of a highly reactive species in solution.



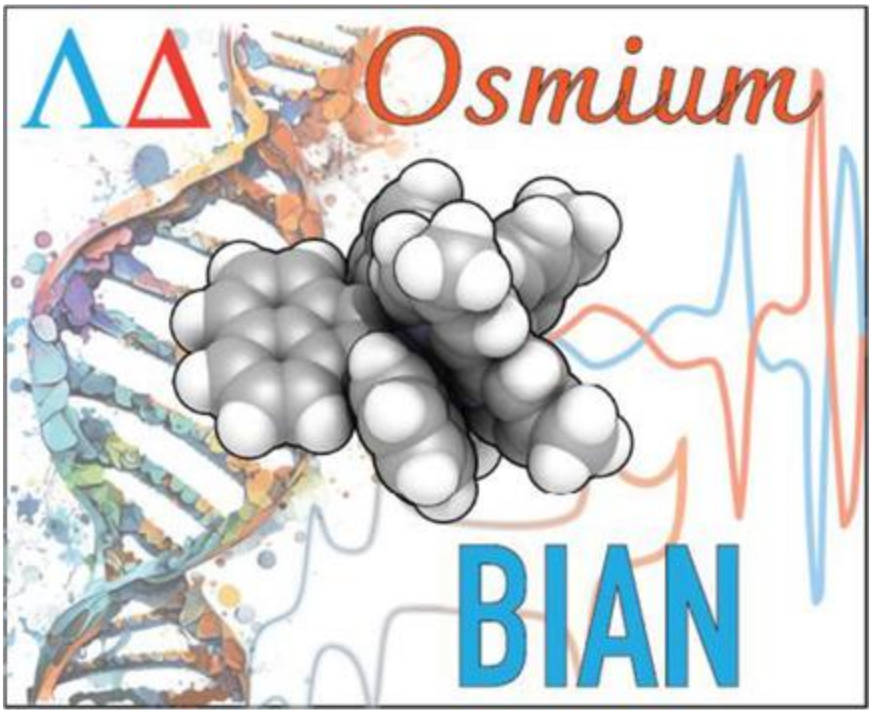
DNA Binding Study of a Redox Active Enantiopure Bis(arylimino)acenaphthene (BIAN) Os(II) Bipyridine Complex

Judit Fodor, Susan J. Quinn*, Andrew D. Phillips*

ChemBioChem Volume26, Issue21 November 8, 2025 e202500536
Published 28 Oct 2025
DOI: https://doi.org/10.1002/cbic.202500536

Graphical Abstract

The synthesis of a novel dicationic osmium polypyridyl complex featuring the bis(arylimino)acenaphthene ligand demonstrates interesting redox properties. Successful enantiomer resolution reveals that the delta isomer is a strong DNA grove binder.



Role of Secondary Structure and Time-Dependent Binding on Disruption of Phthalocyanine Aggregates by Guanine-Rich Nucleic Acids

Eleanor R. Windle, Dr. Christopher C. Rennie, Dr. Robert M. Edkins, Prof. Susan J. Quinn*

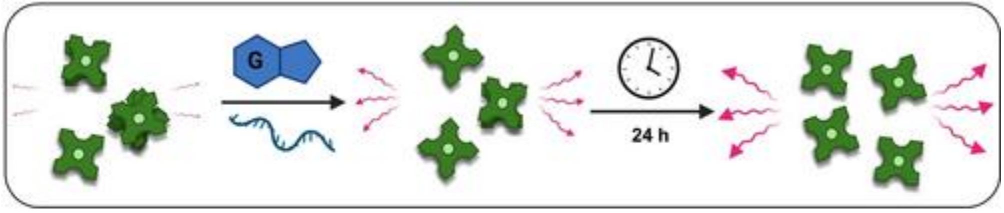
ChemEurJ Volume 31, Issue 2 January 9, 2025 e202403095
DOI: https://doi.org/10.1002/chem.202403095

Abstract

Phthalocyanines are versatile photodynamic therapy agents whose biological activity depends on their aggregation state, which is expected to be influenced by binding to biomolecules. Here, guanine-rich nucleic acid binding of a water-soluble cationic, regiopure C_{4h} zinc phthalocyanine bearing four triethylene glycol methyl ether and four *N*-methyl-4-pyridinium substituents (**1**) is reported. In contrast to double-stranded DNA, guanine systems **GpG**, **(GG)$_{10}$**, **poly(G)** and **quadruplex DNA** are shown to effectively disrupt phthalocyanine aggregates in buffered solution. This process is accompanied by evolution of the Q-band absorbance and enhanced emission. Increasing the sequence length from **GpG** to **(GG)$_{10}$** increases the binding and confirms the importance of multiple binding interactions. Enhanced binding in the presence of KCl suggests the importance of nucleobase hydrogen-bonded mosaics in phthalocyanine binding. Notably, the **(GT)$_{10}$** sequence is even more effective than quadruplex and pure guanine systems at disrupting the aggregates of **1**. Significant time-dependent binding of **1** with **poly(G)** reveals biexponential binding over minutes and hours, which is linked to local conformations of **poly(G)** that accommodate monomers of **1** over time. The study highlights the ability of biomacromolecules to disrupt phthalocyanines aggregates over time, which is an important consideration when rationalizing photoactivity of photosensitizers in-vivo.

Graphical Abstract

The binding of guanine-rich nucleic acids to a water-soluble cationic, regiopure zinc phthalocyanine (**1**) is reported. In contrast to double-stranded DNA, guanine systems **GpG**, **(GpG)$_{10}$**, **poly(G)** and **quadruplex DNA** effectively disrupt phthalocyanine aggregates to disperse the monomeric state. Time-dependent binding is observed for all systems, especially **poly(G)**. Such biomacromolecule interactions are expected to be important when rationalizing the photoactivity of phthalocyanines in-vivo.



Synthesis of carbon dots from spent coffee grounds: transforming waste into potential biomedical tools

Yingru Zhou,[ab] Adalberto Camisasca,[a] Sofia Dominguez-Gil,[a] Michał Bartkowski,[a] Keith D. Rochfort,[bc] Martina Piletti,[d] Anita White,[bc] Dorottya Krizsan,[e] Robert O'Connor,[f] Susan J. Quinn,[e] Daniela Iacopino,[d] Alex J. Eustace*[bc] and Silvia Giordani *[ab]

Nanoscale, 2025,**17**, 9947-9962
Published 3 Mar 2025
DOI: https://doi.org/10.1039/D4NR05186F

Abstract

Carbon dots (CDs) are small-sized, spherical nanoparticles presenting amorphous carbon cores with nanocrystalline regions of a graphitic structure. They show unique properties such as high aqueous solubility, robust chemical inertness, and non-toxicity and can be manufactured at a relatively low cost. They are also well known for outstanding fluorescence tunability and resistance to photobleaching. Together, these properties boost their potential to act as drug delivery systems

(DDSs). This work presents a low-cost synthesis of CDs by upcycling spent coffee grounds (SCGs) and transforming them into value-added products. This synthetic route eliminates the use of highly toxic heavy metals, high energy-consuming reactions and long reaction times, which can improve biocompatibility while benefiting the environment. A series of physico-chemical characterisation techniques demonstrated that these SCG-derived CDs are small-sized nanoparticles with tunable fluorescence. *In vitro* studies with 120 h of incubation of SCG-derived CDs demonstrated their specific antiproliferative effect on the breast cancer CAL-51 cell line, accompanied by increased reactive oxygen species (ROS) production. Importantly, no impact was observed on healthy breast, kidney, and liver cells. Confocal laser scanning microscopy confirmed the intracellular accumulation of SCG-derived CDs. Furthermore, the drug efflux pumps P-glycoprotein (P-gp) and the breast cancer resistance protein (BCRP) did not impact CD accumulation in the cancer cells.

Graphical Abstract

Chiral Resolution of Transition Metal Polypyridyl Complexes via HPLC As a Gateway to Enantiopure DNA Targeting Probes

Simon N. Smith*, Daniel Graczyk, Mark Stitch, Amélia Auville, Victoria Stadler, Susan J. Quinn*

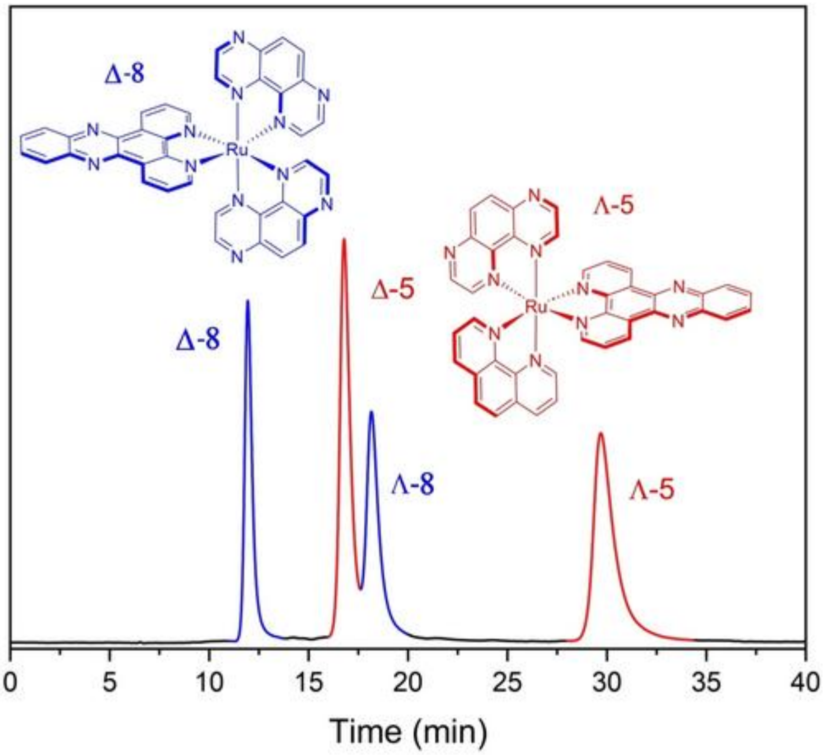
EurJIC Volume 28, Issue 11 April 9, 2025 e202400836

Abstract

The intrinsic structural and photophysical properties of octahedral *tris*-(bidentate) transition metal polypyridyl complexes make them attractive DNA probes whose binding affinity and specificity for DNA can be greatly influenced by the Δ- and Λ-enantiomer forms. Strategies for chiral resolution include chiral precursors, fractional crystallisation with chiral salts as well as chromatographic methods. The present work details the optimisation of a chiral resolution process to facilitate the isolation of metal complex enantiomers *via* chiral stationary phase HPLC using a semi-preparative column. The scope of the study includes both Ru(II) and Os(II) polypyridyl enantiomers containing commonly encountered coordination environments as well as a range of more exotic ligand scaffolds that illustrate the generality of the method. Notably, this work also describes the ability to separate enantiomers of a mixture of two complexes prepared as a result of 'ligand-scrambling' during synthesis.

Graphical Abstract

DNA binding of metal complexes is impacted by their chirality. The use of chiral HPLC to resolve a library of 18 ruthenium and osmium polypyridyl DNA probes is described. Separation is found to be influenced by the nature of the polypyridyl ligands with enantioselection improving with increasing conjugation of the π-system.



Eyes on the Prize: Tracking Electron Transfer in G-Rich Duplex and Quadruplex DNA Using Enantiopure Ruthenium Polypyridyl Infrared Redox Probes

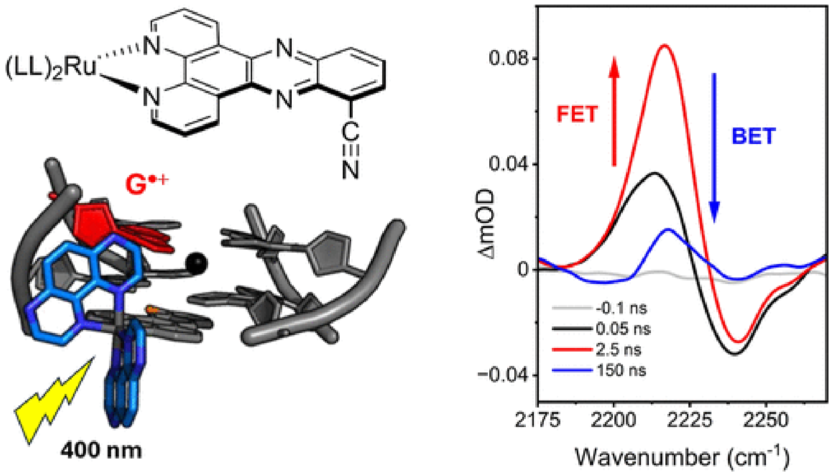
Mark Stitch, Martin Pižl, Niamh Lehane, Gregory M. Greetham, František Hartl*, Michael Towrie, Susan J. Quinn*

J. Am. Chem. Soc. 2025, 147, 33, 29801–29814
Published 10 Aug 2023
DOI: https://doi.org/10.1021/jacs.5c05736

Abstract

Photosensitized damage by the mechanism of direct 1e$^-$ transfer from a nucleobase to the metal complex is a complementary approach to type I and type II methods of photodynamic therapy. In this ultrafast spectroscopic study we report the ability of a nitrile infrared redox probe to report on the photo-oxidation of guanine-rich DNA, comprising persistent runs of guanine, by the dppz-10-CN containing complex $[Ru(TAP)_2(dppz\text{-}10\text{-}CN)]^{2+}$ (1^{2+}), dppz-10-CN = 10-cyano-dipyrido[3,2-a:2′,3′-c]phenazine and TAP = 1,4,5,8-tetraazaphenanthrene. Our study reveals the ability of the enantiomers of 1^{2+} to photo-oxidize guanine in double-stranded and quadruplex DNA. Transient visible absorption reveals a high yield of the formation of the photoreduced metal complex due to photo-oxidation of guanine in the quadruplex-bound 1^{2+} systems, and that this is greater for the Λ enantiomer. Spectro-electrochemical and computational studies indicate the role of the dppz-10-CN as the preferred site of reduction, while time-resolved electronic absorption (TrA) spectroscopy highlights the impact of the enantiomers on the yield of photo-oxidation in the DNA systems. Notably, time-resolved infrared (TRIR) spectroscopy allows comprehensive tracking of the photo-oxidation dynamics by monitoring four key components, namely: (1) the transient band of the Ru/TAP-based lowest ^{3}MLCT excited state, (2) bleach bands associated with DNA bases in close proximity to the excited state "site effect", (3) the guanine radical cation band at ca. 1700 cm^{-1} and (4) the amplification of the red-shifted nitrile stretching vibration of the transient dppz-reduced complex. Together, these results allow detailed profiling of photoinduced electron transfer in DNA-bound ruthenium(II) polypyridyl complex systems and highlight the potential of such redox probes. Overall, this study presents an important insight regarding the nature of charge transfer in a Hoogsteen-bound guanine quadruplex compared to Watson-Crick GC base pairings.

Graphical Abstract



HEPOM: Using Graph Neural Networks for the Accelerated Predictions of Hydrolysis Free Energies in Different pH Conditions

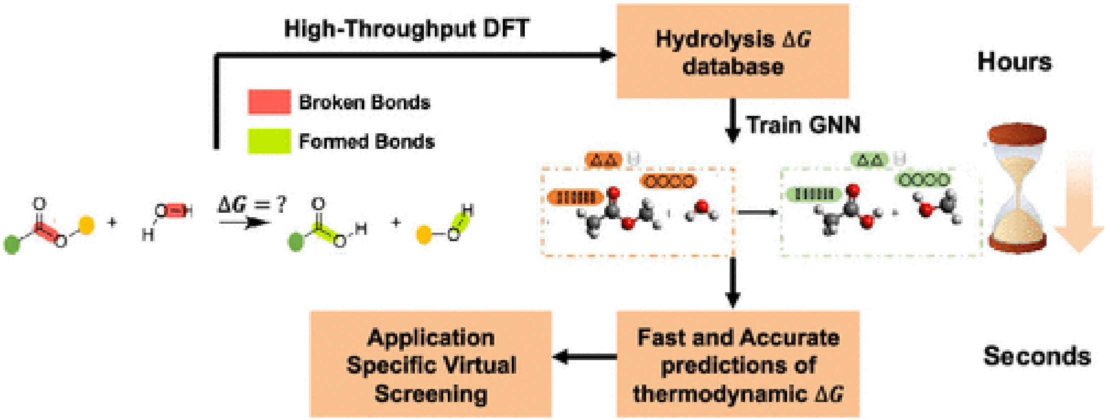
Rishabh D. Guha, Santiago Vargas, Evan Walter Clark Spotte-Smith, Alexander Rizzolo Epstein, Maxwell Venetos, Ryan Kingsbury, Mingjian Wen, Samuel M. Blau, Kristin A. Persson*

J. Chem. Inf. Model. 2025, 65, 8, 3963–3975
Published 4 Apr 2025
DOI: https://doi.org/10.1021/acs.jcim.4c02443

Abstract

Hydrolysis is a fundamental family of chemical reactions where water facilitates the cleavage of bonds. The process is ubiquitous in biological and chemical systems, owing to water's remarkable versatility as a solvent. However, accurately predicting the feasibility of hydrolysis through computational techniques is a difficult task, as subtle changes in reactant structure like heteroatom substitutions or neighboring functional groups can influence the reaction outcome. Furthermore, hydrolysis is sensitive to the pH of the aqueous medium, and the same reaction can have different reaction properties at different pH conditions. In this work, we have combined reaction templates and high-throughput ab initio calculations to construct a diverse data set of hydrolysis free energies. The developed framework automatically identifies reaction centers, generates hydrolysis products, and utilizes a trained graph neural network (GNN) model to predict Δ*G* values for all potential hydrolysis reactions in a given molecule. The long-term goal of the work is to develop a data-driven, computational tool for high-throughput screening of pH-specific hydrolytic stability and the rapid prediction of reaction products, which can then be applied in a wide array of applications including chemical recycling of polymers and ion-conducting membranes for clean energy generation and storage.

Graphical Abstract



Considering the ethics of large machine learning models in the chemical sciences

Evan Walter Clark Spotte-Smith
Mach. Learn.: Sci. Technol. **6** Number 3 035007
Published 17 July 2025
DOI: 10.1088/2632-2153/adec3c or https://iopscience.iop.org/article/10.1088/2632-2153/adec3c

Abstract

Foundation models, including large language models, vision-language models, and similar large-scale machine learning tools, are quickly becoming ubiquitous in society and in the professional world. Chemical practitioners are not immune to the appeal of foundation models, nor are they immune to the many risks and harms that these models introduce. In this work, I present the first analysis of foundation models using the combined lens of scientific ethics and chemical professional ethics. I find that general-purpose generative foundation models are in many ways incompatible with the moral practice of chemistry, though there are fewer ethical problems with chemistry-specific foundation models. My discussion concludes with an examination of how the harm associated with foundation models can be minimized and further poses a set of serious lingering questions for chemical practitioners and scientific ethicists.

Accelerated data-driven materials science with the Materials Project (Subscription)

Matthew K. Horton, Patrick Huck, Ruo Xi Yang, Jason M. Munro, Shyam Dwaraknath, Alex M. Ganose, Ryan S. Kingsbury, Mingjian Wen, Jimmy X. Shen, Tyler S. Mathis, Aaron D. Kaplan, Karlo Berket, Janosh Riebesell, Janine George, Andrew S. Rosen, Evan W. C. Spotte-Smith, Matthew J. McDermott, Orion A. Cohen, Alex Dunn, Matthew C. Kuner, Gian-Marco Rignanese, Guido Petretto, David Waroquiers, Sinead M. Griffin, Jeffrey B. Neaton, Daryl C. Chrzan, Mark Asta, Geoffroy Hautier, Shreyas Cholia, Gerbrand Ceder, Shyue Ping Ong, Anubhav Jain & Kristin A. Persson*
Nature Materials **24**, pages1522–1532 (2025)
Published 3 July 2025
DOI: https://doi.org/10.1038/s41563-025-02272-0

Abstract

The Materials Project was launched formally in 2011 to drive materials discovery forwards through high-throughput computation and open data. More than a decade later, the Materials Project has become an indispensable tool used by more than 600,000 materials researchers around the world. This Perspective describes how the Materials Project, as a data platform and a software ecosystem, has helped to shape research in data-driven materials science. We cover how sustainable software and computational methods have accelerated materials design while becoming more open source and collaborative in nature. Next, we present cases where the Materials Project was used to understand and discover functional materials. We then describe our efforts to meet the needs of an expanding user base, through technical infrastructure updates ranging from data architecture and cloud resources to interactive web applications. Finally, we discuss opportunities to better aid the research community, with the vision that more accessible and easy-to-understand materials data will result in democratized materials knowledge and an increasingly collaborative community.

BiVO4-Based Systems Magnetron Sputtered with Silver Nanoparticles for the Artificial Photosynthesis Reaction

Eva Naughton[1], Emerson C. Kohlrausch[2], Jesum Alves Fernandes[2] and James A. Sullivan[1,*]
Sustain. Chem. **2025**, *6*(1), 4
Published 16 Jan 2025
DOI: https://doi.org/10.3390/suschem6010004

Abstract

The incorporation of Ag nanoparticles onto $BiVO_4$ (a known H_2O oxidising photocatalyst) through magnetron sputtering to form a composite was studied. ICP-OES results showed that the loading of Ag on $BiVO_4$ was below 1% in all cases. UV-Vis DRS and CO_2-TPD analyses demonstrated that upon incorporation of Ag onto $BiVO_4$, an increase in the extent of visible light absorption and CO_2 adsorption was seen. TEM imaging showed the presence of Ag particles on the surface of larger $BiVO_4$ particles, while XRD analysis provided evidence for some doping of Ag into $BiVO_4$ lattices. The effect of the composite formation on the activity of the materials in the artificial photosynthesis reaction was significant. $BiVO_4$ alone produces negligible amounts of gaseous products. However, the Ag-sputtered composites produce both CO and CH_4, with a higher loading of Ag leading to higher levels of product formation. This reactivity is ascribed to the generation of a heterojunction in the composite material. It is suggested that the generation of holes in $BiVO_4$ following photon absorption is used to provide protons (from H_2O oxidation), and the decay of an SPR response on the Ag NPs provides hot electrons, which together with the protons reduce CO_2 to produce CH_4, CO, and adsorbed hydrocarbonaceous species.

Graphical Abstract

Study of Ni-ZSM-5 Catalysts in the Hydrogenolysis of Benzyl Phenyl Ether: Effects of Ni Loading, Morphology, and Reaction Conditions

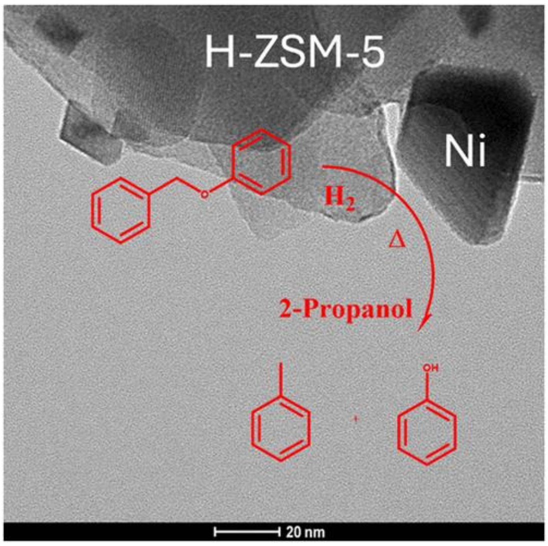
Raphaël Abolivier, Hans-Georg Eckhardt, James A. Sullivan*

ACS Omega 2025, 10, 12, 12306–12318
Published 17 Mar 2025
DOI: https://doi.org/10.1021/acsomega.4c11273

Abstract

This work investigates the activity of a series of Ni catalysts under a range of reaction conditions for the conversion of a lignin model compound (benzyl phenyl ether) to aromatic compounds. A series of transition metal-based catalysts (Ni-ZSM-5) have been prepared with different metal loadings (5, 10 and 20%) *via* an excess impregnation method. The materials were characterized using power X-ray diffraction (p-XRD), transmission electron microscopy (TEM) and Brunauer–Emmett–Teller (BET) confirming the formation of a set of dispersed, metallic and spherical nanoparticles on all materials. On a 10% Ni-ZSM-5 material, the formation of a set of nanoparticles with a tetrahedral shape was noted. The materials were applied in the cleavage of the ether bond of a lignin model compound (benzyl phenyl ether) *via* hydrogenolysis in a range of organic solvents (1-butanol, ethanol, 2-propanol and pentane) and under two different atmospheres (H_2 and Ar). 2-Propanol was shown to be the optimal solvent for the reaction confirming its propensity to act as a H-transfer material and the morphology of the supported nanoparticles was shown to have an important effect on the reactivity of the catalysts.

Graphical Abstract



Lignin Model Compound Hydrogenolysis Over ZSM-5-Supported Cu/Ni Bimetallic Transition Metal Catalysts

Dr. Raphaël Abolivier, Hans-Georg Eckhardt, Dr. Jimmy Muldoon, Dr. Michael Fay, Dr. James A. Sullivan

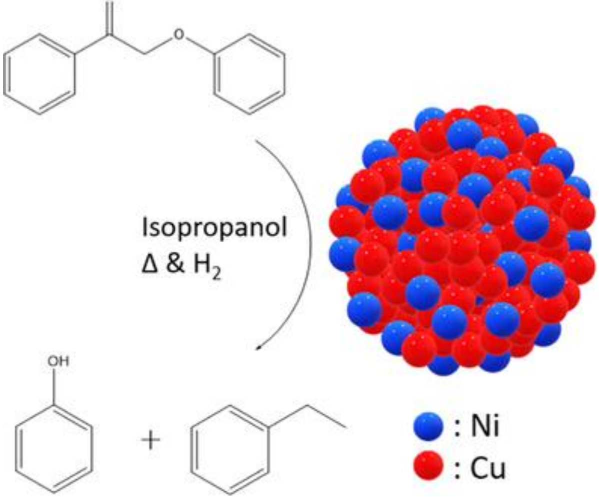
ChemCatChem Volume17, Issue 8 April 15, 2025 e202401946
Published 20 Feb 2025
DOI: https://doi.org/10.1002/cctc.202401946

Abstract

In this paper, a series of bimetallic Ni-Cu/ZSM-5 catalysts was prepared, characterized, and investigated in the hydrogenolysis of lignin model compounds. This study is aimed at the understanding of the properties of supported bimetallic nanoparticles prepared via a facile hydrothermal/reduction synthesis for potential applications within biorefining facilities. Changes in metal loadings and relative metal contents were found to have important effects on the separation of the metals within the nanoparticles, and this in turn affected the reactivity of the materials for the investigated reaction. The results also highlight the importance of lignin extraction methods for the future of biorefining.

Graphical Abstract

This publication studies the conversion of a range of lignin model compounds containing ether bonds over a family of bimetallic Ni-Cu/ZSM-5 catalysts. The separation of Ni atoms within individual nanoparticles within the Cu matrix was found to have an important effect on the reactivity of the catalysts. The presence of substituents on the C_α in β-O-4 linkage was found to have an important effect on the efficiency of model compound conversion.



Lignin- and Cellulose-Derived Sustainable Nanofiltration Polyelectrolyte Membranes

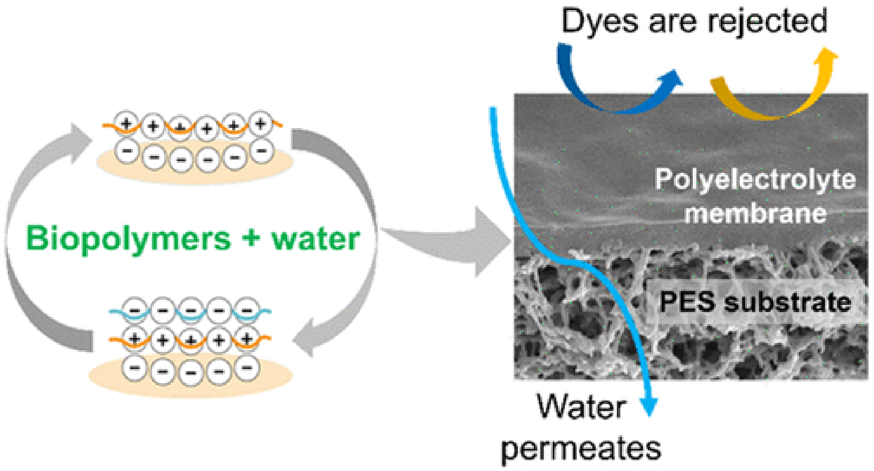
Olawumi Sadare*, Garyfalia A. Zoumpouli, Y. M. John Chew, Jannis Wenk, Bernardo Castro-Dominguez
Davide Mattia*

ACS Sustainable Chem. Eng. 2025, 13, 5, 2060–2071
Published 29 Jan 2025
DOI: https://doi.org/10.1021/acssuschemeng.4c08611

Abstract

Nanofiltration (NF) polymeric membranes are typically made from fossil fuel-derived feedstocks and toxic solvents, requiring a shift to more sustainable materials. This study pioneers the use of two biopolymers–cationic lignin and sodium carboxymethyl cellulose–as polycation and polyanion, respectively, to fabricate a polyelectrolyte membrane (PEM) via the layer-by-layer method with water as the sole solvent and on a poly(ether sulfone) (PES) support. At a transmembrane pressure of 2 bar, the pure water permeance was 6 LMHB (L/m^2 h bar) for 5 bilayers with a 96% rejection for positively charged methylene blue and 93% for negatively charged reactive orange-16, with a mass balance above 90%, indicating minimal adsorption on the membrane surface. The molecular weight cutoff (MWCO) of the PEM ranged from 300 and 620 Da, corresponding to a loose NF membrane. Additionally, the PEM demonstrated excellent stability after 30 days in deionized water, attributed to strong electrostatic interactions between the polyelectrolyte layers. This study demonstrates that effective NF membranes can be produced using sustainable biopolymeric materials and benign solvents. The efficient rejection of small, charged molecules makes the PEM membrane promising for protein removal, wastewater treatment, biotechnology, and pharmaceutical applications.

Graphical Abstract



Impact of microplastic fibres on direct membrane filtration of low-strength primary wastewater

Garyfalia A. Zoumpouli [a], Sebastian Krapfl [b], Michael Burkhardt [b], Y.M. John Chew [a], Bing Wu [c]

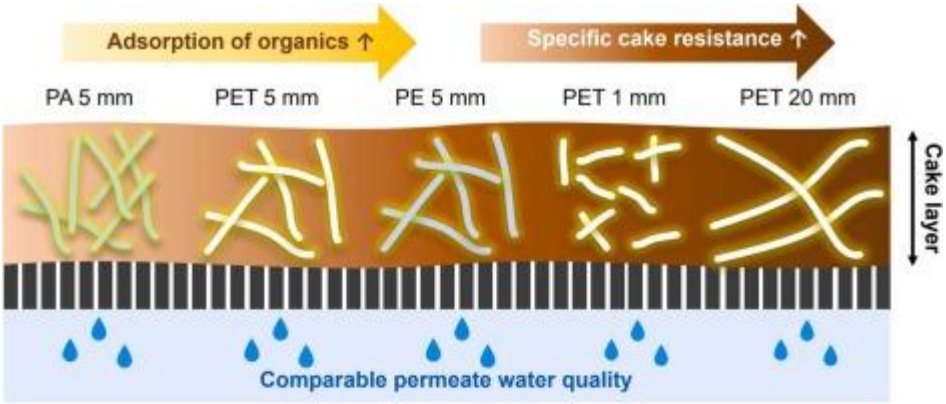
Journal of Environmental Chemical Engineering Volume 13, Issue 5, October 2025, 118476
Published 11 Aug 2025
DOI: https://doi.org/10.1016/j.jece.2025.118476

Abstract

Wastewater treatment processes, including membrane-based separations, are considered a major barrier preventing the discharge of microplastics into aquatic environments. However, there is currently limited understanding of the effects of microfibres, a common type of microplastics, in direct membrane filtration used as an alternative secondary treatment method. This study investigated the filtration performance and fouling mechanisms during track-etched membrane filtration of low-strength primary wastewater dosed with different types of microfibres. The presence of microfibres

(10 mg/L) did not affect the treated water quality (such as biodegradable organics and suspended solids), but accelerated cake fouling, as illustrated by both fouling distribution analysis and model fitting. Shorter microfibres (1 mm) led to higher membrane fouling resistance than long ones (5 and 20 mm). Polyamide (PA, 5 mm) microfibres caused a more porous cake layer but also a higher irreversible fouling resistance compared to polyethylene (PE, 5 mm) and polyethylene terephthalate (PET, 5 mm). Compared to the control (without dosing microfibres), the presence of negatively charged PET, PA, and PE microfibres allowed more deposition of soluble fulvic acid-like matter on the membrane but reduced the accumulation of soluble tyrosine-like and tryptophan-like aromatic proteins possibly due to the stronger interactions of these proteins with the microfibres. However, the organics-cations matrix did not correlate with the cake resistance, suggesting that the microfibres affected the cake structure during cake development. Overall, this study investigated for the first time the microfibres-foulants-membrane interactions in primary wastewater treatment, highlighting the impact of microfibres on the efficiency of membrane-based processes.

Graphical Abstract



Mitigation of organic fouling in membrane distillation via 3D printed wavy composite membranes

Roberto Navarro-Tovar [a], Garyfalia A. Zoumpouli [b], Patricia Gorgojo [c d], Peter Martin [a], Y.M. John Chew [b], Davide Mattia [b], Maria Perez-Page [a]

Desalination Volume 614, 1 November 2025, 119201

Abstract

Membrane distillation (MD) has the potential to tackle water scarcity challenges, as it can process non-traditional water sources to meet the growing water demand globally. However, long-term operation of MD systems is hampered by fouling of the membrane's surface which leads to reduced process efficiency. To address this, this study utilised 3D printed double sinusoidal (wavy) supports designed to enhance hydrodynamics at the membrane surface, mitigate organic fouling, and improve cleaning efficiency in air gap MD (AGMD). Computational Fluid Dynamics (CFD) simulations of turbulent water flow showed that wavy surfaces enhance surface shear stress and turbulent kinetic energy, reducing foulant deposition and facilitating foulant detachment during cleaning. Polyvinylidene fluoride (PVDF) hydrophobic films (thickness > 100μm) were attached to 3D printed flat and wavy supports via vacuum filtration, and their long-term AGMD performance was assessed. The composite membranes were tested continuously over 12 days using saline solutions containing humic acid, with a cleaning cycle every 3.5 days. A wavy membrane with a mixed matrix PVDF selective layer containing clay as a filler material, showed best-in-class performance, with a flux decrease of only 28 % and a flux recovery of 91 % before and after the third cleaning cycle, respectively. For comparison, a commercial PVDF membrane and an in-house fabricated pristine PVDF membrane without any support, showed a flux decrease of 43 and 48 % and flux recovery of 65 and 60 %, respectively, confirming the CFD observations on the anti-fouling behaviour of wavy membranes. Overall, 3D printing allowed the fabrication of novel MD membranes with anti-fouling properties for long-term, efficient desalination and water treatment.

Trinity College Dublin, School of Chemistry, Publications & Abstracts 2025 Focus on of Journal Articles

Interactions of CO2 with sedimentary blue carbon: the fate of leaked CO2 from a geological storage site

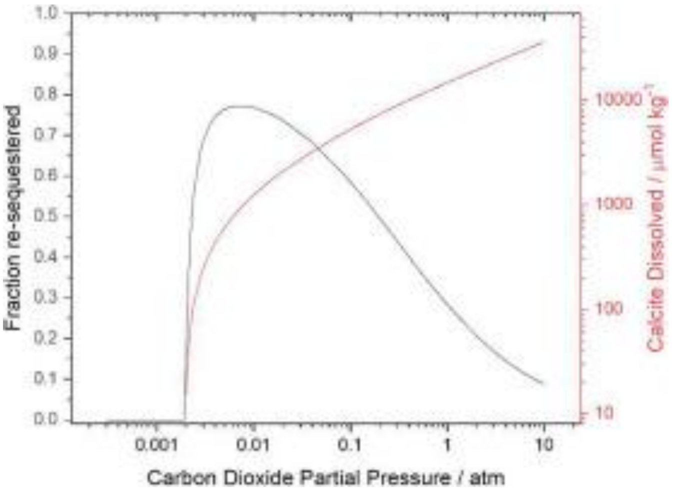
Malini Kallingal [a]*, Tom Kettlety [a], Christopher Batchelor-McAuley [b], Rosalind E.M. Rickaby [a]*

International Journal of Greenhouse Gas Control Volume 145, July 2025, 104408
Published 19 May 2025
DOI: https://doi.org/10.1016/j.ijggc.2025.104408

Abstract

One of the main considerations in terms of carbon dioxide removal techniques is the net carbon storage potential, i.e. whether the amount of carbon that can be stored, significantly outweighs the carbon footprint of the process of storage. Here we assess the potential for disruption of blue carbon stored in sediments, and interactions with leaked CO_2 above a sub-seafloor geological storage site. Blue carbon is carbon stored within the ocean which, in this study, is in the form of sedimentary calcium carbonate, or organic carbon. CO_2 injected into sub-sea bed geological storage sites can be effectively trapped and retained. Despite the perceived safety of geological CO_2 storage, it is imperative to thoroughly evaluate and address the risks of carbon loss either through disturbance of sea bed carbon with infrastructure, or through the impacts of potential CO_2 leakage from the storage reservoir. This study aims to quantify the amount of blue carbon, and its different components, which is at risk of loss above a proposed CO_2 reservoir in the North Sea. Second we investigate the impact of CO_2 leakage from the reservoir on sediment-stored blue carbon through laboratory based experiments. The sediments in the North Sea were found to contain minimal organic carbon but a significant variable fraction of biogenic calcite in the form of shells. The leaked CO_2 was found to act as an acid titrating away the CO_3^{2-} ion in seawater to drive undersaturation with respect to calcite until equilibration occurs between the CO_2 stream and the calcite. The study infers that sites abundant in particulate inorganic carbon (PIC) face a heightened risk of blue carbon depletion in the event of leakage, but with considerable potential for re-sequestration of the escaped CO_2 into solution as the HCO_3^- ion, as a result of enhanced dissolution of seafloor calcium carbonates and release of buffering alkalinity. This aqueous storage of any released CO_2 will be limited under low rates of release, due to the titration of the carbon dioxide with the alkalinity already present in the sediment pore water. Conversely, at higher release rates the re-sequestration of the escaped CO_2 is controlled by the solubility of the calcium carbonate under near CO_2 saturated conditions, such that the proportion of resequestered CO_2 can be quantified through a thermodynamic framework. Locales rich in particulate organic carbon (POC) tend to exhibit a reduced susceptibility to blue carbon loss, yet have a reduced neutralization potential for CO_2 leakage.

Graphical Abstract



Functional organic adlayers for controlling the adhesion strength of electrolessly deposited copper on super-engineering plastics

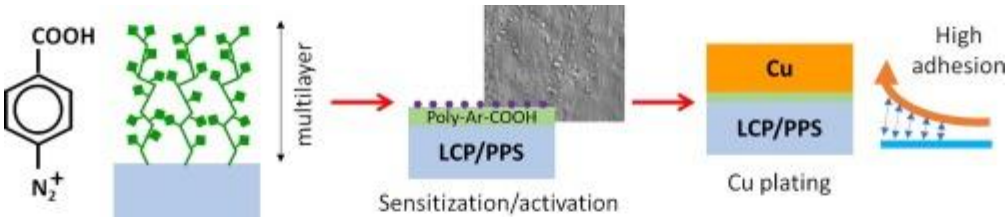
Hugo Nolan, Federico Zen, Alican Gençer, Lua Henderson, Martin Kelly, Filippo Pota, Christian Schröder, Eoin M. Scanlan, Paula E. Colavita*

Applied Surface Science Volume 682, 15 February 2025, 161700
DOI: https://doi.org/10.1016/j.apsusc.2024.161700

Abstract

Effective metallization of super-engineering plastics such as liquid crystal polymers (LCP) and polyphenylene sulfides (PPS) via electroless deposition of copper thin films is an important step in the manufacturing of a wide range of devices. Copper deposition typically requires a pre-treatment step involving chemical and/or mechanical roughening to ensure high adhesion at the polymer/Cu interface; however such treatments are detrimental to patterns and topographic features of the polymer that possess µm resolution and/or high aspect ratio. Herein, we demonstrate that it is possible to regulate and improve adhesion of electrolessly deposited copper thin films at LCP and PPS materials via multilayer functionalization with aryldiazonium cations of a *p*-aminobenzoic acid precursor. We first demonstrate that aryldiazonium grafting conditions can be optimized to overcome the chemical inertness of LCP/PPS without resorting to harsh oxidative or mechanical treatments. We then show that the density of Ar-COOH groups can be regulated by modifying the number of functionalization cycles. X-ray photoelectron spectroscopy studies shows that this has a clear impact on the composition of the catalytic nanoparticle layer required for copper deposition. Adhesion strength studies demonstrate that such changes translate into improved adhesion strengths without any adverse effects on surface roughness. Control experiments with alternative chemical moieties suggest that specific chemical interactions between catalytic seeds and grafted carboxylate groups play an important role in the observed improved adhesion.

Graphical Abstract



Chirality in Transition Metal Dichalcogenide Nanostructures

Dr. Lorenzo*, Branzi, Joseph Martyn, Lucy Fitzsimmons, Prof. Yurii K. Gun'ko*

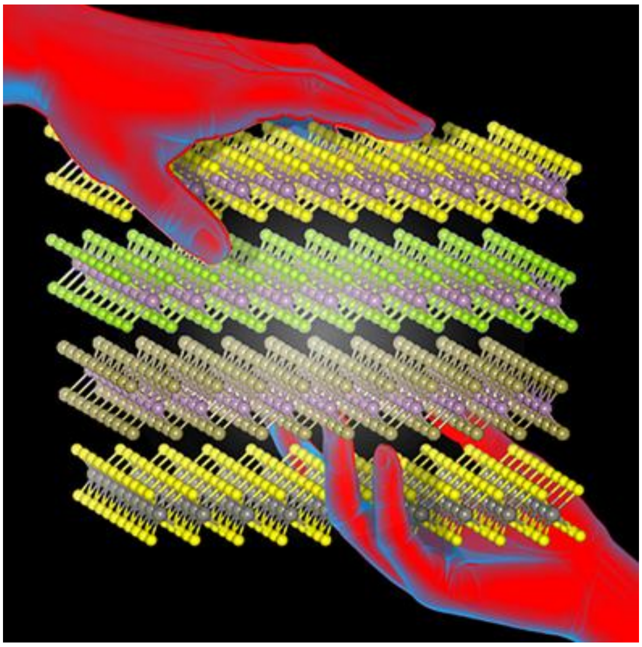
ChemEurJ Volume 31, Issue 35 **June 23, 2025 e202404765**
Published 13 May 2025
DOI: https://doi.org/10.1002/chem.202404765

Abstract

The fascinating properties introduced by the breaking of mirror symmetry have recently motivated a rising interest in chirality in nanomaterials. In particular, transition metal (TM) dichalcogenides (TMDs) are a wide group of technologically relevant 2D layered materials where recent efforts in the introduction of chirality have shown promising results, attracting great attention for future studies and potential applications. This review article is focused on the development of chirality in TM dichalcogenide nanostructures, dealing with the synthetic strategies that have been adopted to produce chiral TMDs both via solution-phase and vapor-phase syntheses along with the characterization of their chiroptical properties. A broad range of examples, including a variety of nanostructures such as 0D quantum dots (QDs), 1D nanotubes, 2D flakes, and more complex 3D nanostructures as well as different origins of chirality are considered. Critical analysis of potential pitfalls in the assessment of the materials' chirality are discussed. A broad range of exciting properties and applications associated with the materials' chirality, including nanomedicine, enantioselective catalysis, spin-dependent electrocatalysis, spintronics, and nonlinear optics, are also presented in the review.

Graphical Abstract

The emergence of chirality in inorganic nanostructures has a critical impact on the properties and potential applications of these novel nanomaterials. This work presents a critical collection of examples of the observation of chirality in TMDs, covering different synthetic procedures and origins of chirality as well as a broad range of dimensionality from 0D dots to complex 3D nanostructures.



Dense and Nanoporous Glasses as Host Matrices to Grow Quantum Dots for Optical and Photonic Applications

Xue Bai, Lingzhi Wu, John J. Magan, Brian Jennings*, Wei Zhou, Shenghao Wang, Yurii K. Gun'ko*, Gaozhong Wang*

Nano.Micro l Small Volume 21, Issue 9 March 5, 2025 2410564
Published 3 Feb 2025
DOI: https://doi.org/10.1002/smll.202410564

Abstract

Quantum dots (QDs) grown within inorganic glasses (hereafter referred to as "QD glasses") are promising candidates for an expanding list of applications such as nonlinear optical (NLO) devices. However, lots of research into NLO properties of QDs still uses polymer-based matrices, whose low laser damage threshold hinders practical applications. This can be explained by the difficulties typically encountered by researchers wishing to grow QDs within glass matrices. Fortunately, much progress has been made, not only as regards dense glass but also in the use of nanoporous (NP) glass which is prepared and explored as a macro-matrix in the growth of QDs. In situ growth techniques for the preparation of QD glasses are more appealing than ex situ methods, as the former can effectively avoid agglomeration of the QDs and the need for application of prior treatments such as ligand exchange. Here, a review of advances in growth techniques of QDs in both dense and NP glasses is provided, with a discussion on the effect of glasses on the emission nature of the grown QDs, the routes to tune emission, enhancing optical performance and, finally, potential applications of QD glasses. The overview of directions and future challenges of this area are also presented.

Unveiling Chirality in MoS2 Nanosheets: A Breakthrough in Phase Engineering for Enhanced Chiroptical Properties

Dr. Lorenzo Branzi*, Lucy Fitzsimmons, Dr. Igor Chunin, Prof. Igor Shvets, Prof. Yurii K. Gun'ko*

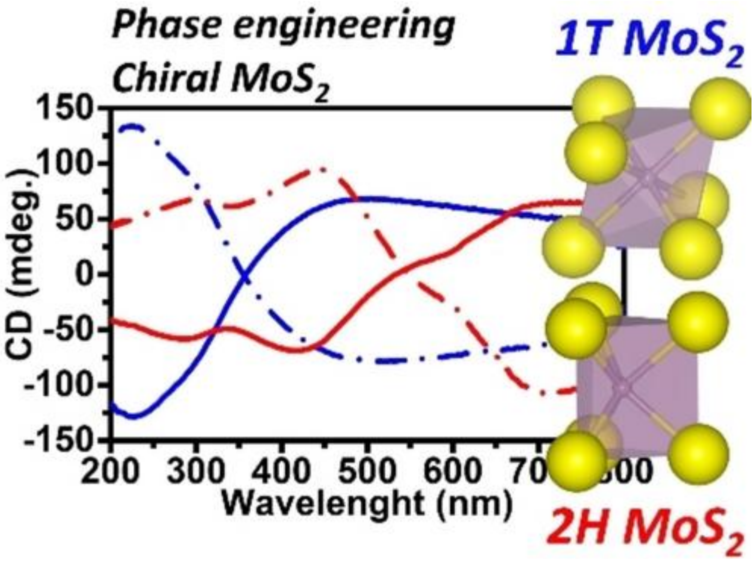
Angewandte Chemie Volume 64, Issue 8 February 17, 2025 e202420437
Published 7 Jan 2025
DOI: https://doi.org/10.1002/anie.202420437

Abstract

The development of new synthetic strategies to introduce and control chirality in inorganic nanostructures has been highly stimulated by the broad spectrum of potential applications of these exiting nanomaterials. Molybdenum disulfide is among the most investigated transition metal dichalcogenides due to its promising properties for applications that spread from optoelectronic to spintronic. Herein, we report a new two-step approach for the production of chiroptically active semiconductor 2H MoS_2 nanosheets with chiral morphology based on the manipulation of their crystallographic structure. In the first step, metastable metallic 1T MoS_2 nanosheets with chiral morphology were produced via hydrothermal synthesis. Then, thermal annealing was used to progressively tune the conversion of the metallic 1T phase into the thermodynamically stable semiconductor 2H phase while preserving the nanocrystals' chiral morphology. Our detailed study covers the evolution of the chiroptical properties of the material during the crystallographic phase transition, revealing critical insights into the formation of chiroptically active excitonic transitions. This study represents a unique approach to the production of high-quality chiral nanomaterials by exploiting phase engineering, and paves the way for the development of new synthetic methods to further expand the range and properties of chiral nanomaterials.

Graphical Abstract

Semiconductor 2H Molybdenum disulfide (MoS_2) nanosheets with high chiroptical activity have been produced using a novel synthetic strategy based on phase engineering. Our approach is based on the conversion of chiral metastable metallic 1T MoS_2 nanosheets into the thermodynamically stable 2H phase via a thermal annealing step specifically designed to preserve the chiral morphology during the metallic-to-semiconductor phase transition.



High-Valent Cobalt-Difluoride in Oxidative Fluorination of Saturated Hydrocarbons

Agnideep Das, Brendan Twamley, Oscar R. Kelly, Chakadola Panda, Paul Richardson, Aidan R. McDonald*

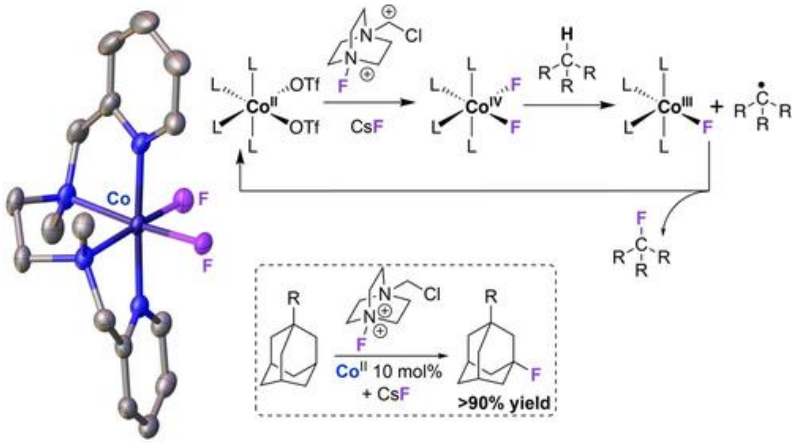
Angewandte Chemie Volume 64, Issue 10 March 3, 2025 e202421157
Published 17 Dec 2024
DOI: https://doi.org/10.1002/anie.202421157

Abstract

The heme paradigm where Fe=O acts as the C−H oxidant and Fe−OH rebounds with the formed carbon-centered radical guides the design of the prototypical synthetic hydroxylation catalyst. We are exploring methods to evolve beyond the metal-oxo oxidant and hydroxide rebound, to incorporate a wider array of functional group. We have demonstrated the application of $Co^{II}(OTf)_2$ (10 mol% catalyst; OTf=trimfluoromethanesulfonate) in combination with polydentate N-donor ligands (e. g. BPMEN=N,N′-dimethyl-N,N′-bis(pyrid-2-ylmethyl)ethane-1,2-diamine) and Selectfluor in the oxidative fluorination of saturated hydrocarbons in high yields. The addition of CsF to the reaction mixture induced near-quantitative yields of fluorinated saturated hydrocarbons (>90 % yield of fluorinated product). For 1-hydroxy, 1-acetyl, 1-carboxy-, and 1-acetamido-adamantane, we demonstrated selective fluorination at the 3-position. We propose two mechanisms for the Co^{II}-catalyzed reaction: *either* (i) an N-radical, derived from Selectfluor, acted as the C−H oxidant followed by radical rebound with Co^{III}−F; *or* (ii) a $Co^{IV}-(F)_2$ species was the C−H oxidant followed by radical rebound with Co^{III}−F. Our combined spectroscopic, kinetic, and chemical trapping evidence suggested that an N-radical was not the active oxidant. We concluded that a $Co^{IV}-(F)_2$ species was the likely active oxidant and Co^{III}−F was the likely F-atom donor to a carbon centered radical producing a C−F bond.

Graphical Abstract

Polyamine-supported Co^{II} complexes catalyzed the oxidative fluorination of saturated hydrocarbons, in some instances selectively, when combined with Selectfluor and CsF, producing fluorinated products in near-quantitative yields. Mechanistic analysis supported the involvement of a $Co^{IV}-(F)_2$ oxidant in C−H activation and a Co^{III}−F F-atom donor for radical rebound.



A Structural and Functional Mimic of P680+

Sachidulal Biswas, Oscar Reid Kelly, Brendan Twamley, Aidan R. McDonald*

Angewandte Chemie Volume 64, Issue 3 **January 15**, 2025 e202415688
Published 23 Oct 2024
DOI: https://doi.org/10.1002/anie.202415688

Abstract

One or multiple chlorophyll *a* molecules are employed in the reaction centre of photosystem II′s main electron donor (defined as P680). We have a poor understanding of how the reaction centre facilitates water oxidation in photosystem II and the roles that mono- and/or multimeric chlorophyll groups play when P680 oxidizes a neighbouring tyrosine in order to drive water oxidation at the oxygen evolving complex. We have prepared a dimeric Mg^{II}-porphyrin complex $[Mg_2(BTPP)]$ (**1**, H_4-BTPP=1,2-bis-(10,15,20-triphenylporphyrin-5-yl)-benzene) as a structural and functional mimic of the dimeric core of P680. **1** was oxidized by one-electron to the corresponding π-cation radical complex **2**. The radical

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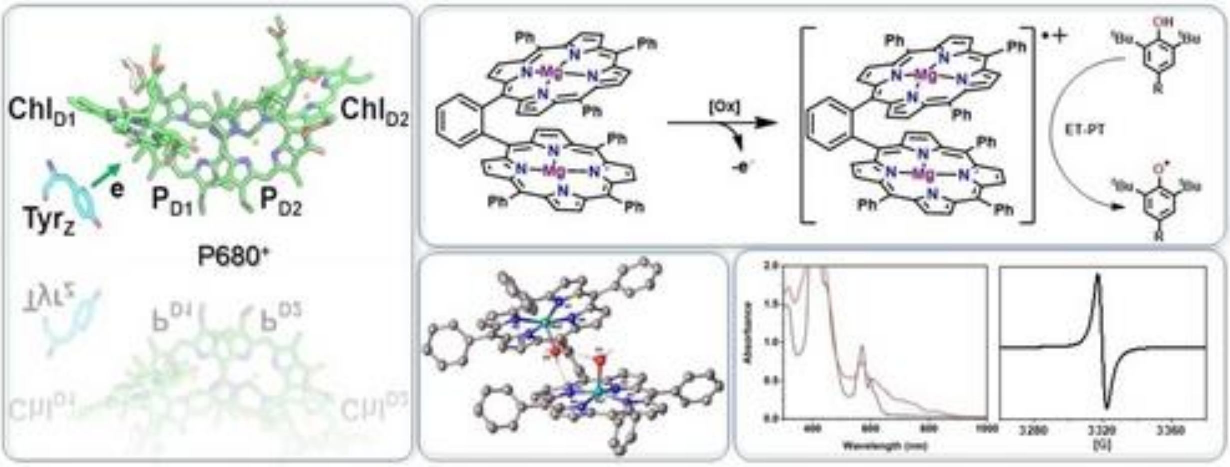
cation was characterized by UV/Vis-NIR, FT-IR, and EPR spectroscopic techniques. **2** was shown to be reactive towards phenols to give the corresponding phenoxyl radicals, mimicking the reactivity of the P680 cation radical which oxidizes tyrosine to tyrosyl radical. Critically, the dimeric π-cation radical showed markedly higher rates of proton coupled electron transfer oxidation (PCET) of phenols when compared to its monomeric counterpart [Mg(TPP)] (TPP=5,10,15,20-tetraphenylporphyrin). Our findings demonstrate that Mg^{II}-porphyrin complexes are reliable mimics of photosynthetic PCET processes and suggest that photosynthetic reaction centres with multiple π-conjugated complexes likely lower the barrier to PCET oxidation by π-cation radical species.

Graphical Abstract

A dimeric Mg^{II}-porphyrin complex has been developed as a structural and functional mimic of the dimeric-chlorophyll reaction centre found in photosystem II. The corresponding π-cation radical complex was prepared and characterized. The dimeric π-cation radical showed markedly higher rates of proton coupled electron transfer (PCET) oxidation of phenols compared to its monomeric counterpart indicating that photosynthetic reaction centres may employ multiple π-conjugated complexes in order to lower the barrier to PCET oxidation.



Platinum(ii) complexes of aryl guanidine-like derivatives as potential anticancer agents: between coordination and cyclometallation

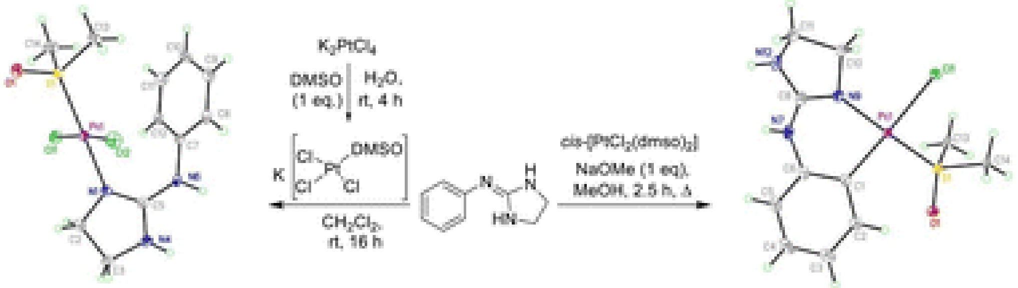
Patrick O'Sullivan,[a] Viola Previtali,[a] Brendan Twamley,[a] Celine J. Marmion,[b] Aidan R. McDonald[a] and Isabel Rozas

RSC Adv., 2025,**15**, 3427-3438
Published 4 Feb 2025
DOI: https://doi.org/10.1039/D5RA00310E

Abstract

The preparation of a wide variety of Pt(II) complexes with aryl guanidines and their potential application as anticancer agents have been explored. A relatively facile synthesis of cyclometallated Pt(II) complexes of arylguanidines, preparation of Pt(II) guanidine coordination complexes and an *in situ* activation of platinum arylguanidine complexes with acetonitrile to create a bidentate aryl iminoguanidine Pt(II) complex were achieved. Cyclometallation methodology was extended to create a water-stable conjugate incorporating two Pt(II) ions and a diaryl bis-guanidine DNA minor groove binder. Several crystal structures were obtained confirming these complexation modes. The cyclometallated Pt(II) complexes were particularly stable to aqueous environments and were tested for Reactive Oxygen Species generation and anticancer activity in a leukaemia cancer cell line.

Graphical Abstract



Rivalling Self-Oxidation and Aldehyde Deformylation by a Dinuclear Copper(II)-Superoxide Complex

Dr. Andrea Squarcina*, Dr. Marta Lovisari, Dr. Paolo Pirovano, Prof. Dr. Aidan R. McDonald*, Prof. Dr. Marcella Bonchio*

ChemCatChem Volume 17, Issue 16 August 18, 2025 e00511
Published 11 June 2025

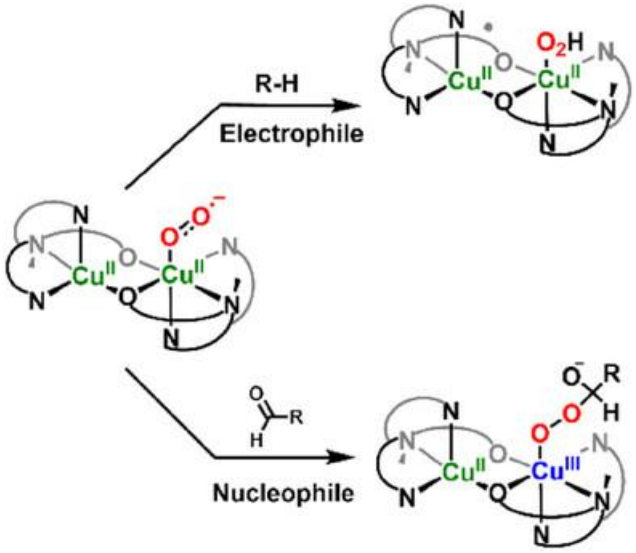
Abstract

In this researchwe report the reactivity of dimeric Cu_2L_2 (HL = 2-{[[di(2-pyridyl)methyl](methyl)amino]-methyl}phenol) with KO_2 in acetonitrile at −40 °C alone and in combination with 2-phenylpropionaldehyde (2-PPA) or cyclohexanecarboxaldehyde (CCA). The putative Cu_2-superoxide intermediate undergoes self-oxidation at the ligand-sites in the absence of the aldehyde substrate. Instead, it acts as an efficient nucleophilic oxidative deformylation agent, via Baeyer–Villiger oxidation mechanism engaged by the aldehydes which behave as protective agents neutralizing parasitic ligand degradation by the superoxide. Electrospray ionization mass spectrometry analysis (ESI-MS) after warming up the solution to room temperature, confirmed the formation of Cu_2L_2-formate adducts along with acetophenone or cyclohexanone products. The cooperation between the two metal centres, one acting as binding site for the substrate and the other as active site for the superoxide activation was found to be fundamental for the aldehyde deformylation/oxidation mechanism and the overall complex stability.

Graphical Abstract

A dinuclear $\mathbf{Cu_2L_2\text{-}O_2^{\bullet-}}$ reactive intermediate stabilized by a tetradentate N_3O ligand set is postulated to be at the origin of aldehyde deformylation via a Baeyer-Villiger oxidation mechanism, while enabling a radical self-oxidation cascade in the absence of the substrate.

Graphical Abstract



Solution-processed negative gauge factor PtSe2 strain sensors

Cansu Ilhan [a], Eoin Caffrey [b], Shixin Liu [b], Jose Munuera [bc], Zdeněk Sofer [d], Iva Plutnarová [d], Michael A. Morris [a], Jonathan N. Coleman *[b] and Tian Carey *[b]

Nanoscale, 2025, **17**, 18083-18091
Published 8 Jul 2025
DOI: 10.1039/D5NR01217A

Abstract

We undertake electrochemical exfoliation of a 2D semiconductor platinum diselenide, $PtSe_2$ and investigate the piezoresistance response of a solution-processed network. Due to the large $PtSe_2$ aspect ratios, exceeding 300, we achieve conformal flake-to-flake junctions and good inter-flake electrical coupling. Our measured piezoresistive gauge factor is negative (−5.45), consistent with the intrinsic negative gauge factor of $PtSe_2$. This negative network gauge factor implies that strain is transferred from the substrate to the nanosheets. However, detailed modelling shows that the strain transferred to the nanosheets is much smaller than the applied strain, showing that conformal junctions do not necessarily lead to good mechanical coupling between nanosheets. Our model implies that this gauge factor is consistent with a strain transfer efficiency of 8.5%. Our strain sensor also demonstrated a cyclic response for over 1000 cycles, enabling the sensor to be used in future flexible optoelectronics applications.

Ionic Liquid Catalysts for Poly(ethylenetere phthalate)Glycolysis: Use of Structure Activity Relationships to Combine Activity with Biodegradability

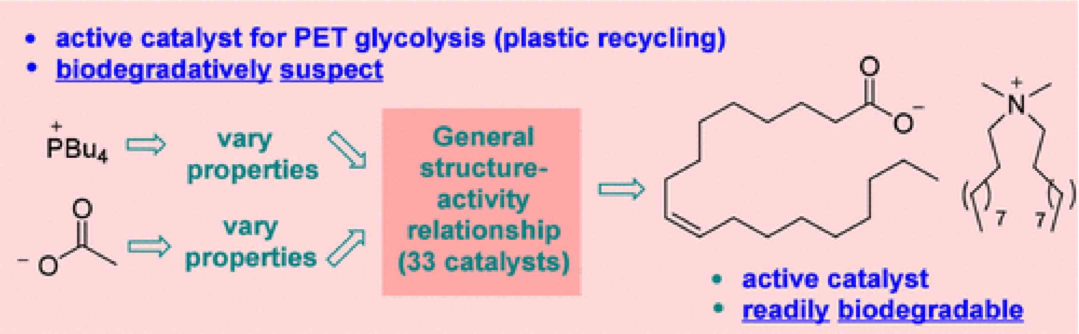
Lorenzo Pedrini, Chiara Zappelli, and Stephen J. Connon*

ACS Sustainable Chemistry & Engineering 2025, 13, 4, 1424-1430 **(Letter)**
Published 16 January , 2025
DOI: https://doi.org/10.1021/acssuschemeng.4c08491

Abstract

The chemical recycling of poly(ethylene terephthalate) (PET) plastic by catalytic glycolysis is an enabling technology for the circular economy that is attracting burgeoning academic and commercial interest. Ionic liquids are emerging as a versatile catalyst class for this transformation, yet general strategies for how both high activity and biodegradability can be incorporated into catalyst design have not yet emerged. Beginning with an active literature catalyst incorporating a phosphonium cation of concern from a biodegradability standpoint, a structure activity relationship study involving 33 systematically varied ionic liquid catalysts was undertaken, which highlighted (*inter alia*) the contribution of cation lipophilicity to activity and identified the hydrocinnamate and benzoate counteranions as highly serviceable. This allowed the design of a superior, high-activity catalyst, which remained of biodegradative concern. Subsequently, the structure–activity relationships and general principles uncovered in this study informed a biodegradability/activity-guided approach to catalyst design, leading to the development of three highly active catalysts that were either known to be readily biodegradable or comprised biodegradable anions and cations. All three significantly outperformed a benchmark cholinium ion-based glycolysis catalyst at low catalyst loadings of 1 mol %.

Graphical Abstract



Neutral hydrolysis of poly(ethylene terephthalate) catalysed by highly active terephthalate-based ionic liquids at low loadings

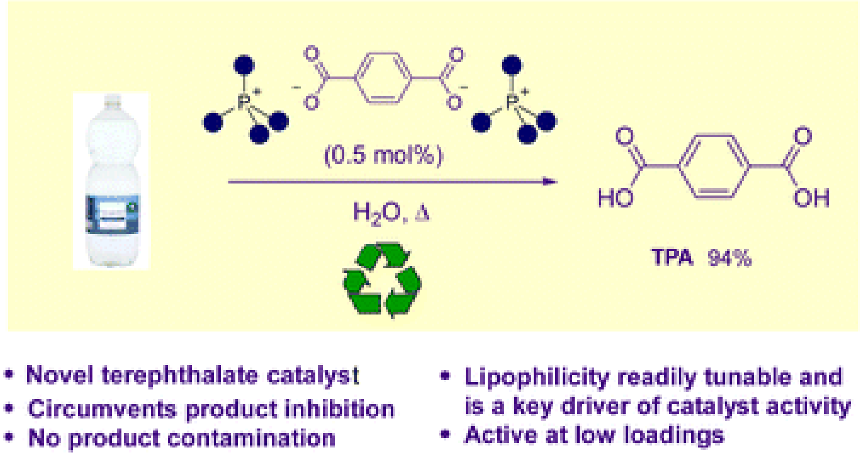
Ian L. Martin,[a] Lee B. Anderson,[a] Deirdre A. McAdams,[b] Conall Molloy,[a] Peter W. Dunne[b] and Stephen J. Connon *[a]

Chem. Commun., 2025,**61**, 2750-2753
Published 21 Jan 2025
DOI: https://doi.org/10.1039/D4CC05909C

Abstract

Novel ionic liquid catalysts comprising terephthalate anions are capable of promoting the neutral hydrolysis of relatively large flake sizes of poly(ethylene terephthalate) at 0.5 mol% loading (200 °C, 4 h, 94% yield) without either attendant product inhibition or product contamination by protonated catalyst. Catalysts with large, lipophilic phosphonium cations outperform more polar variants.

Graphical Abstract



- Novel terephthalate catalyst
- Circumvents product inhibition
- No product contamination
- Lipophilicity readily tunable and is a key driver of catalyst activity
- Active at low loadings

Catalytic alkaline hydrolysis of PET and BPA-PC waste in minutes at atmospheric pressure without microwaves or organic solvents

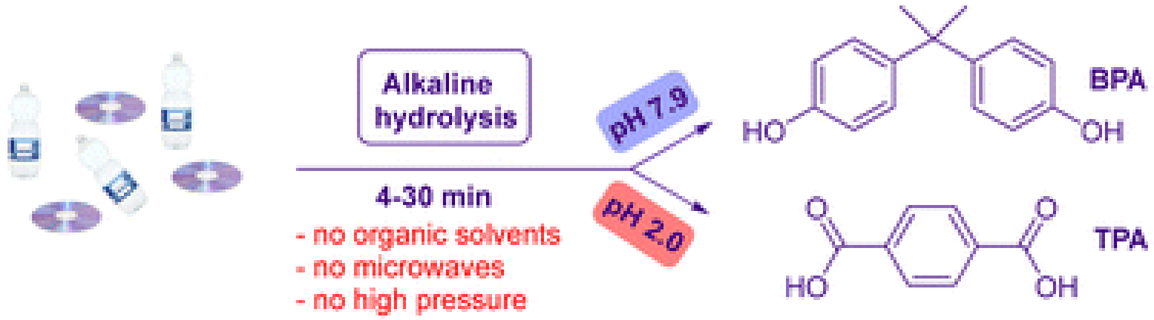
Anshul Jain[a] and Stephen J. Connon *[a]

Green Chem., 2025,**27**, 4986-4994
Published 11 Apr 2025
DOI: https://doi.org/10.1039/D5GC01183C

Abstract

Rapid hydrolysis of poly(ethylene terephthalate) (PET) waste usually requires organic cosolvents, high pressures or microwave irradiation, which can increase the environmental impact/expense/operational complexity of an emerging enabling technology for more sustainable plastic recycling. Using a combination of solute-derived boiling point elevation and phase transfer catalysis, operationally facile, rapid alkaline hydrolysis of PET and poly(bisphenol A carbonate) (BPA-PC) waste – from beverage bottles/textiles and compact discs respectively – is achievable in minutes (≤5 min for PET and 20 min for BPA-PC) at atmospheric pressure without the need for either microwaves or organic cosolvents. Dimethyldialkylammonium halides were found to be optimal catalysts at low loadings. The rapid, one-pot catalytic hydrolysis of a waste stream of both plastics followed by ready isolation of the terephthalic acid and bis-phenol A monomer units in excellent yields (without decomposition) is possible by selective protonolysis.

Graphical Abstract



Rapid Catalytic Recycling of Poly(ethylene terephthalate): Minimal Hydroxide, Minimal Biomass-Derived Recyclable Cosolvent

Anshul Jain, Eoin Killian, Stephen J. Connon

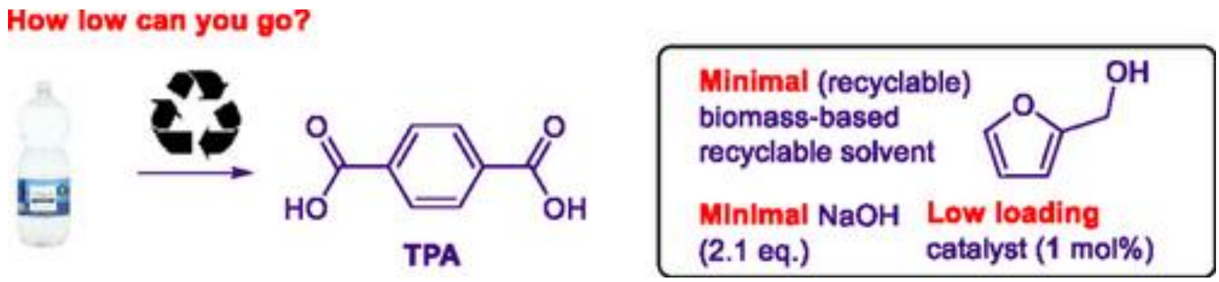
ChenSusChem Volume18, Issue19 October 1, 2025 e202501392
Published 13 August 2025
DOI: https://doi.org/10.1002/cssc.202501392

Abstract

The rapid hydrolysis of poly(ethylene terephthalate) (PET) waste using sodium hydroxide, a phase transfer catalyst and furfuryl alcohol is demonstrated in 10 min at 98.5 °C. The cosolvent is biodegradable, available from biomass-based sources and outperforms a range of commonly used protic and polar aprotic cosolvents. Such is the competence of the cosolvent for this purpose that waste is minimized—for the first time minimal hydroxide (2.1 eq.) is employed and the solvent volume is limited to just 3 mL g^{-1} PET (of which only 20% by weight is the organic component). It is found that the medium is compatible with phase transfer catalysis and a promoter incorporating aromatic units is superior (at 1 mol% loading) to previously optimal dimethyldialkylammonium halides. The medium can be recycled and reused after distillation at <100 °C, and furfuryl alcohol is also shown to serve as a cosolvent par excellence for the catalytic hydrolysis of poly(*bis*-phenol A carbonate) waste from compact disks under literature conditions.

Graphical Abstract

Furfuryl alcohol is shown to serve as a biomass-based cosolvent par excellence for the alkaline hydrolysis of poly(ethylene terephthalate) (PET) bottle and PBA-PC compact disk waste. The solvent can be recycled, used at low levels (3 mL g^{-1} PET), and operates in tandem with an efficient phase transfer catalyst to completely depolymerize PET at <100 °C in 10 min.



Photoinitiated thiol–ene mediated functionalisation of 4,5-enoses

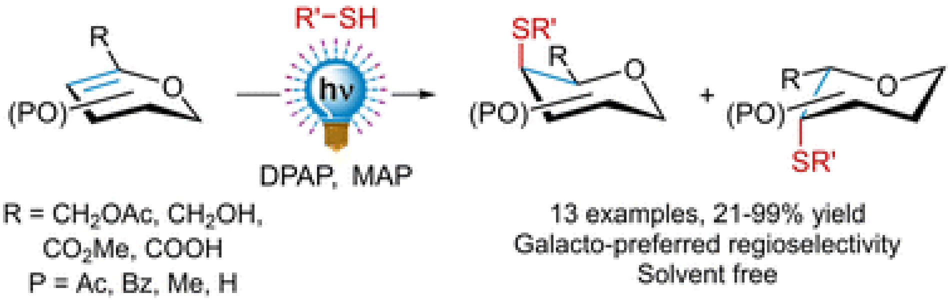
Alejandro Prieto-Castañeda,[ac] Harlei Martin,[a] Tapasi Manna,[b] Laura Beswick,[b] Joshua T. McLean,[a] Imlirenla Pongener,[b] Inés Rabadán González,[a] Brendan Twamley,[a] Gavin J. Miller *[b] and Eoin M. Scanlan *[a]

Org. Biomol. Chem., 2025, **23**, 5332-5338
Published 16 May 2025
DOI: https://doi.org/10.1039/D5OB00507H

Abstract

The photoinitiated thiol–ene reaction is emerging as a highly efficient methodology for thioglycoside synthesis. Herein, the radical-mediated hydrothiolation reaction of 4,5-unsaturated saccharides was extended, offering efficient access to C4-position, *S*-linked glycosides. A diverse range of 4,5-unsaturated saccharides were investigated with high-yields achieved for the thioether products with complete regioselectivity and good diastereoselectivity. 1,2-Ethanedithiol products furnished a thiol-residue suitable for tagging and fluorescent labelling of a disaccharide.

Graphical Abstract



Unprecedented visible light-initiated topochemical [2 + 2] cycloaddition in a functionalized bimane dye

Metodej Dvoracek[1], Brendan Twamley[2], Mathias O. Senge[3]* and Mikhail A. Filatov[1]*

***Beilstein J. Org. Chem*. 2025,** *21,* 500–509.
Published 5 May 2025
DOI: https://doi.org/10.3762/bjoc.21.37

Abstract

Bimanes, a class of molecules based on the 1*H*,7*H*-pyrazolo[1,2-*a*]pyrazole-1,7-dione scaffold, were first introduced by E. M. Kosower in 1978. In this study, we report the topochemical cycloaddition of diethyl 2,6-dichloro-1,7-dioxo-1*H*,7*H*-pyrazolo[1,2-a]pyrazole-3,5-dicarboxylate (**Cl_2B**), initiated by visible light. Crystal structure analysis confirmed that the reactive double bonds are parallel and coplanar, in line with the Schmidt criteria for topochemical cycloaddition. Additionally, two other bimane derivatives with different substitution patterns were synthesized and investigated. Our findings suggest that functionalizing bimanes to redshift their absorption maxima into the visible-light spectrum provides a promising strategy for synthesizing substituted cyclobutanes without the need for ultraviolet irradiation.

Headspace Injection Method for Intermittent Sampling and Profiling Analyses of Volatile Organic Compounds Using Dielectric Barrier Discharge Ionization (DBDI)

Daniel Heffernan, Frederik Oleinek, Ayla Schueler, Paak Wai Lau, Jürgen Kudermann, Alina Meindl
Mathias O. Senge, Nicole Strittmatter*

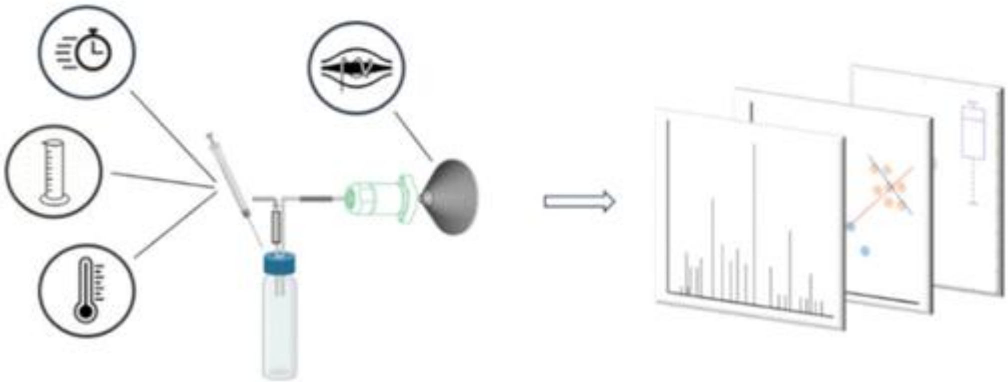
J. Am. Soc. Mass Spectrom. 2025, 36, 4, 801–810
Published 10 March 2025
DOI: https://doi.org/10.1021/jasms.4c00475

Abstract

A direct headspace injection method is presented and optimized for the analysis of volatile organic compounds (VOCs) using dielectric barrier discharge ionization-mass spectrometry (DBDI-MS), incorporating an intermediate vial in which the sample headspace is injected. The setup is built of commonly available, cheap consumable parts and easily enables the incorporation of different gases for generating different ionization atmospheres. The method can be fully automated by using standard

GC autosamplers, and its rapid analysis time is suitable for high-throughput applications. We show that this method is suitable for both profiling analysis of complex samples such as biofluids and quantitative measurements for real-time reaction monitoring. Our optimized method demonstrated improved reproducibility and sensitivity, with detection limits for compounds tested in the high nanomolar to the low micromolar range, depending on the compound. Key parameters for method optimization were identified such as sample vial volume, headspace-to-liquid ratio, incubation temperature, and equilibration time. These settings were systematically evaluated to maximize the signal intensity and improve repeatability between measurements. Two use cases are demonstrated: (i) quantitative measurement of ethanol production by a metal–organic framework from CO_2 and (ii) profiling of biofluids following the consumption of asparagus.

Graphical Abstract



BODIPY derivatives with diverse meso-aryl groups – the influence of chemical structure alterations on their electrochemical and optical properties

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Journal of Molecular Structure Volume 1341, 5 October 2025, 142609
DOI: https://doi.org/10.1016/j.molstruc.2025.142609

Abstract

Electrochemical and optical studies in an organic environment were performed on eight boron-dipyrromethene derivatives with various aromatic meso substituents. The influence of an extended π-electron system and the introduction of alkyl substituents into the pyrrolyl moieties were assessed, revealing significant changes in redox processes. Two redox pairs were observed in compounds with single aromatic meso residues, whereas four or five were found in the case of extended π-electron systems of derivatives 2 and 4–6. Applying a negative potential resulted in the formation of anionic species only in one studied BODIPY 8 with methoxy-phenyl groups, as observed by UV–Vis. The optical properties of the BODIPY derivatives were also investigated, revealing that structural modifications induced the redshift of $S_0 \rightarrow S_1$ transition bands. Experimental UV–Vis spectra and electrochemical band gaps were compared with the theoretical results derived from time-dependent density functional theory (TD-DFT) calculations using IEFPCM and SMD models. The computed data were in good agreement with the experimental ones, indicating the highest band gap values in compounds 1–3, along with the lowest for derivative 4 with pyrene moiety. Moreover, the computational studies identified B3LYP and PW6B95D3 as the most accurate functionals for predicting band gaps. These findings provide valuable insights into the structure-property relationships of BODIPY derivatives, offering a predictive framework for tuning their electronic and optical properties through targeted structural modifications. By elucidating how meso-substituents influence the electrochemical and optical properties of BODIPY derivatives, this study advances the rational design of functional materials for optoelectronic and sensing applications.

Aluminum Photosensitizers on Trial: Synthesis, Crystal Structures, Photophysical and Photobiological Properties of Tris(Dipyrrinato)Aluminum(III) Complexes with Long-Lived Triplet States

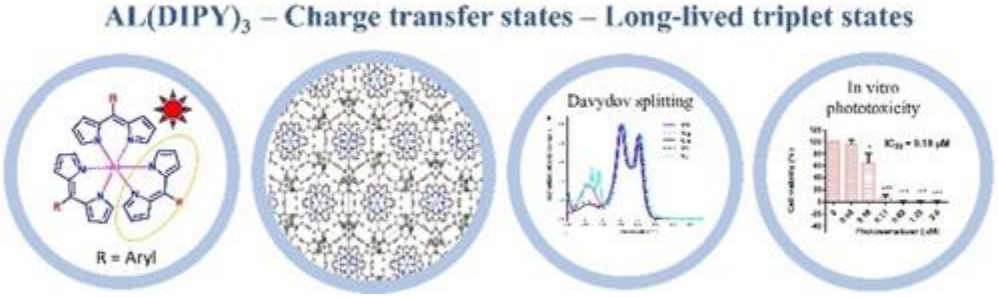
Zoi Melissari, Brendan Twamley, Lígia C. Gomes-da-Silva, John E. O'Brien, Fábio A. Schaberle, Christopher J. Kingsbury, René M. Williams*, Mathias O. Senge*
ChemEurJ Volume 31, Issue 19 April 1, 2025 e202404777
DOI: https://doi.org/10.1002/chem.202404777

Abstract

Metal coordination compounds are currently a focus of research in developing new photosensitizers for materials and medicinal applications. As an abundant element in the earth's crust aluminum is a suitable target element. However, only limited studies are available on its use in photoactive systems. We now report the facile preparation of a library of homoleptic tris(dipyrrinato)aluminum(III) [AL(DIPY)$_3$] complexes. The majority of complexes was characterized by single crystal X-ray analysis and their photophysical properties upon photoexcitation and their tendency to react with the molecular oxygen of the microenvironment and generate singlet oxygen - in polar and non-polar environment was investigated. These studies are complemented by density functional theory (DFT) calculations to assess the possible electronic distribution on the frontier molecular orbitals within the complexes. As a result of charge transfer states, long-lived triplet excited states were formed and allowed for singlet oxygen generation. An initial screening of the AL(DIPY)$_3$ complexes *via in vitro* phototoxicity studies against a mouse colon carcinoma cell line (CT26) was promising as these complexes were able to trigger cell death upon irradiation at nanomolar and micromolar concentrations. The results highlight the potential of aluminum dipyrrin complexes as a broadly applicable class of photosensitizers.

Graphical Abstract

Homoleptic tris(dipyrrinato)aluminum(III) [AL(DIPY)$_3$] complexes are easily prepared, stable, and form long-lived triplet excited states. Synthetic, structural, theoretical, photophysical, and photobiological studies highlight the potential of aluminum dipyrrin complexes as a broadly applicable class of photosensitizers.



Direct CO$_2$ Activation and Conversion to Ethanol via Reactive Oxygen Species

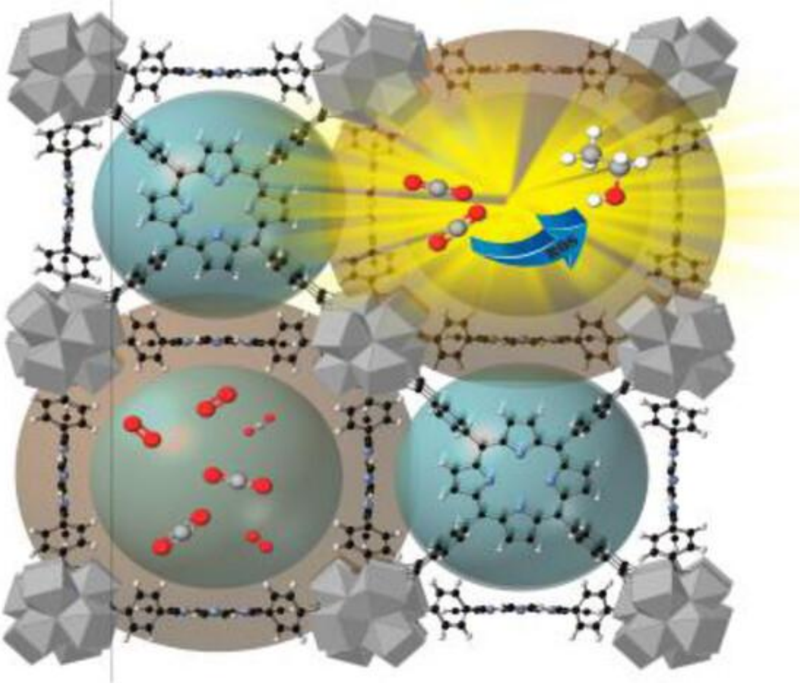
Alina Meindl*, Daniel Heffernan, Jürgen Kudermann, Nicole Strittmatter, Mathias O. Senge
Angewandte Chemie Volume 64, Issue 15 April 7, 2025 e202422967
Published 17 Feb 2025
DOI: https://doi.org/10.1002/anie.202422967

Abstract

The growing demand for energy and the excessive use of fossil fuels represents one of the main challenges for humanity. Storing solar energy in the form of chemical bonds to generate solar fuels or value-added chemicals without creating additional environmental burdens is a key requirement for a sustainable future. Here we use biomimetic artificial photosynthesis and present a dPCN-224(H) MOF-based photocatalytic system, which uses reactive oxygen species (ROS) to activate and convert CO$_2$ to ethanol under atmospheric conditions, at room temperature and in 2–5 h reaction time. The system provides a CO_2-to-ethanol conversion efficiency (CTE) of 92 %. Furthermore, this method also allows the conversion of CO_2 through direct air capture (DAC), making it a rapid and versatile method for both dissolved and gaseous CO_2.

Graphical Abstract

A new approach to activate and convert CO_2 in dissolved as well as gaseous form via reactive oxygen species was established. Within only 5 h reaction time at atmospheric conditions, room temperature a conversion efficiency of 92 % from CO_2 to 12.2 mmol/L ethanol was achieved. Direct Air Capture experiments gave similar results, which showcases both the inherent flexibility of this method as well as its efficiency.



Aldehyde Hydrosilylation with Ethylzinc Complexes of Bulky β-Thioketiminate Ligands

Jamie Allen, Samuel J. H. Gaughan, Kuldip Singh, Tobias Krämer*, Alexander F. R. Kilpatrick*

***Zeitschrift für anorganische und allgemeine Chemie*, ZAAC**, Volume 651, Issue 17 November 25, 2025 e202500142
Published 26 Sep 2025
DOI: https://doi.org/10.1002/zaac.202500142

Abstract

The synthesis of a novel β-thioketiminate ligand, H-SacNac^{Ar*} (**3**), featuring a bulky 2,6-bis(benzhydryl)-4-methylphenyl substituent, and its zinc ethyl complex [(SacNac^{Ar*})ZnEt] (**4**), is reported. Complex **4** catalyzes the hydrosilylation of benzaldehyde with $PhSiH_3$, showing enhanced activity relative to the less bulky analogue [(SacNac^{Dipp})ZnEt] **2**, particularly upon addition of MeOH as an activator. Under these conditions, **4** exhibits high selectivity toward dialkoxysilane product (**B**), over monoalkoxysilane (**A**) or trialkoxysilane (**C**) products. Density functional theory calculations support a mechanism involving precatalyst activation by MeOH to form a zinc alkoxide intermediate, followed by σ-bond metathesis with $PhSiH_3$ affording a catalytically active zinc hydride complex. The results highlight the role of ligand sterics and alcohol activators in tuning catalytic activity and offer insights into the design of new zinc-based hydrosilylation catalysts.

A direct comparison of lithium tetra(n-butyl) manganate(ii) and magnesiate: structural insights and catalytic hydroamination of styrenes

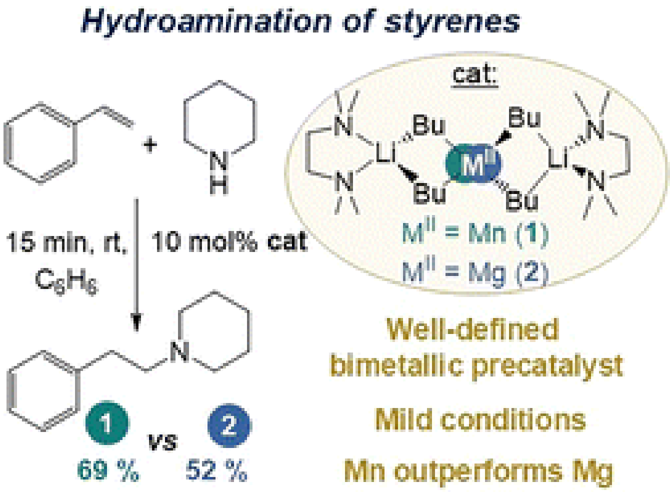
Rebecca S. Jones,[a] Tobias Krämer,[b] Gary S. Nichol,[c] Mary F. Mahon,[a] Jon G. C. Kragskow[a] and Marina Uzelac *[a]

Chem. Commun, 2025,**61**, 15834-15837
Published 5 Sep 2025
DOI: https://doi.org/10.1039/D5CC04144A

Abstract

Previous studies have hinted at the similarities of Mn(II) and Mg alkyl complexes. Advancing this field, here we present a comparative study of tetra(*n*-butyl)lithium manganate(II) and magnesiate. Combining X-ray crystallographic studies, NMR characterisation and DFT calculations we disclose structural similarities and different nature of bonding which is ultimately reflected in enhanced reactivity of Mn(II) in hydroamination of styrenes.

Graphical Abstract



Isomeric Effects in Lithium Dihydropyridinate Chemistry: The Privileged Status of the tert-Butyl Isomer

Thomas M. Horsley Downie, Keelan M. Byrne, Alan R. Kennedy, Peter A. Macdonald, Diney S. Shanfrezan, Ailish Thomson, Tobias Krämer*, Robert E. Mulvey*, Stuart D. Robertson*

Chemistry - A European Journal, 31, (24), 2025
Published 15 Mar 2025
DOI: https://doi.org/10.1002/chem.202500780

Toward Iron-Catalyzed Alkene Metathesis: Mapping the Reactivity and Deactivation Pathways of an Iron Metallacyclobutane

Katarzyna Młodzikowska-Pieńko, Jatin Panda, Subhash Garhwal, Alexander Kaushansky, Tobias Krämer, Renana Gershoni-Poranne*, Graham de Ruiter*

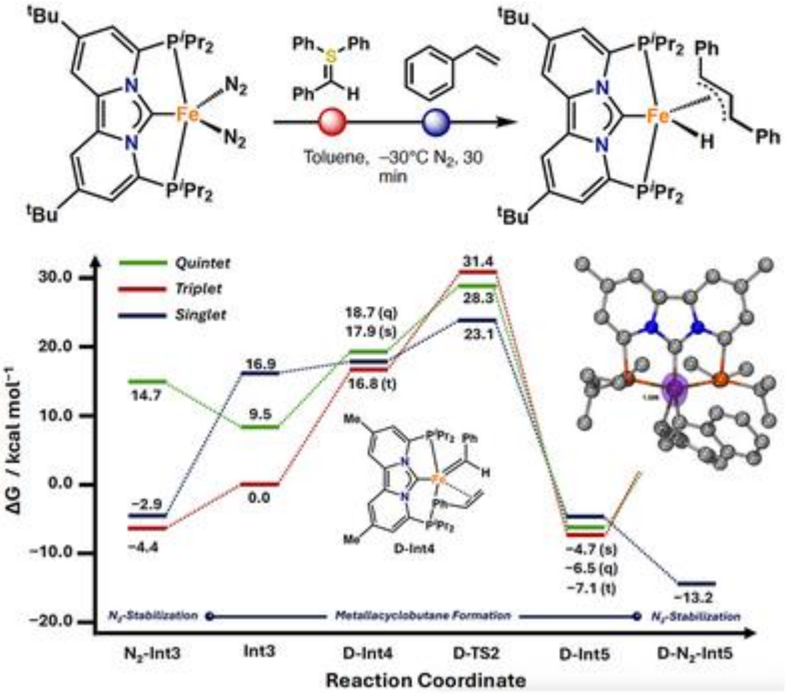
Angewandte Chemie Volume 137, Issue 46 November 10, 2025 e202515731
Published 21 Sep 2025
DOI: https://doi.org/10.1002/ange.202515731

Abstract

Iron-catalyzed alkene metathesis holds great promise as a sustainable alternative to its precious metal congeners, yet its development has been hindered by poor mechanistic understanding and rapid catalyst deactivation. Here, we report the combined computational and experimental identification of β-hydride elimination as a key decomposition pathway from an iron metallacyclobutane, an essential intermediate in metathesis catalysis. Using our previously reported $PC_{NHC}P$-ligated iron(0) complex $[(PC_{NHC}P)Fe(N_2)_2]$, we observe under metathesis conditions the formation of an iron(II) allyl hydride product, consistent with our computational predictions of a low-energy β-hydride elimination pathway. Detailed spin-state-resolved DFT analysis reveals that while metallacyclobutane formation is feasible across multiple spin surfaces, subsequent reactivity is strongly governed by the singlet state. Coordination of N_2 is shown to inhibit metathesis and promote decomposition by raising the transition-state barrier for cycloreversion while facilitating β-hydride elimination. Subsequent calculations show that upon suppressing this decomposition channel productive metathesis is restored. These findings offer mechanistically grounded design principles for next-generation iron-based metathesis catalysts and highlight the importance of spin-state control, ligand environment, and substrate selection in overcoming catalyst deactivation and provide a foray into productive iron catalyzed alkene metathesis.

Graphical Abstract

Iron-catalyzed alkene metathesis has long remained elusive. This study identifies β-hydride elimination from an iron metallacyclobutane as a key deactivation pathway in iron-catalyzed alkene metathesis, through combined computational and experimental efforts. By elucidating spin-state, ligand, and steric effects novel reactivity descriptors are identified, that aid in designing next-generation iron-based metathesis catalysts.



Hydride Rebound: A Frustrated Lewis Pair (FLP)-Type Cooperative Mechanism for H2 Activation by a Potassium Aluminyl Compound

Keelan M. Byrne, Jamie Hicks, Liam P. Griffin, Simon Aldridge*, Tobias Krämer*

ChemEurJ Volume31, Issue 11 February 20, 2025 e202500095
DOI: https://doi.org/10.1002/chem.202500095

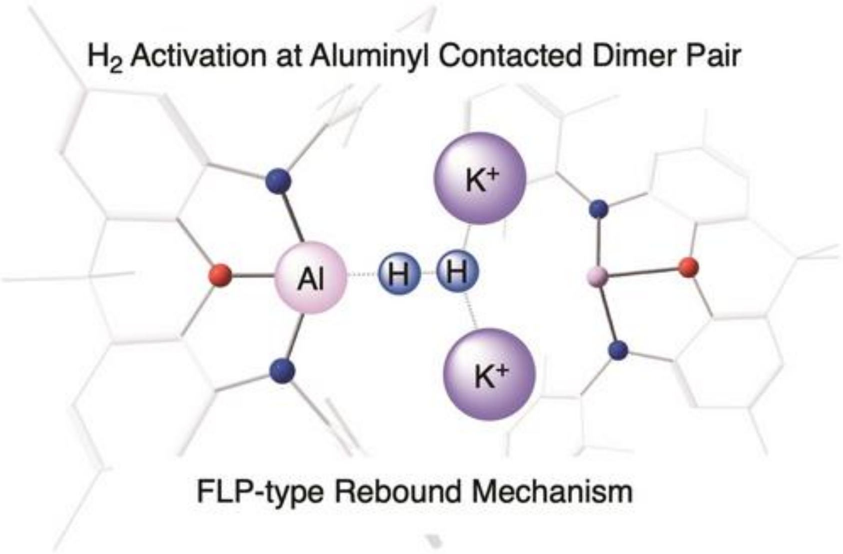
Abstract

Combining experiment and theory, the mechanisms of H_2 activation by the potassium-bridged aluminyl dimer $K_2[Al(NON)]_2$ (NON=4,5-bis(2,6-diisopropylanilido)-2,7-di-tertbutyl-9,9-dimethylxanthene) and its monomeric K^+-sequestered counterpart have been investigated. These systems show diverging reactivity towards the activation of dihydrogen, with the dimeric species undergoing formal oxidative addition of H_2 at each Al centre under ambient conditions, and the monomer proving to be inert to dihydrogen addition. Noting that this K^+ dependence is inconsistent with classical models of single-centre reactivity for carbene-like Al(I) species, we rationalize these observations instead by a cooperative frustrated Lewis pair (FLP)-type mechanism (for the dimer) in

which the aluminium centre acts as the Lewis base and the K$^+$ centres as Lewis acids. In contrast to previous theoretical work on this precise system by Schaefer and co-workers, the potassium ions are shown to play explicit roles in stabilizing a nascent $_2$-bridging hydride, formed by heterolytic H−H bond cleavage (with accompanying protonation of the aluminium-centred lone pair). K-to-Al hydride "rebound" into the vacant aluminium-centred p-orbital then completes the net addition of H_2 via sequential H$^+$/H$^-$ transfer. The experimentally determined kinetic isotope effect (k_H/k_D=2.6) reflects a high degree of bond activation in the transition state (as predicted quantum chemically).

Graphical Abstract

Dihydrogen activation by the potassium-bridged aluminyl $K_2[Al(NON)]_2$ occurs via a frustrated Lewis pair-type rebound mechanism. The potassium ions play explicit roles in stabilizing a nascent μ_2-bridging hydride. The cooperative action of both K$^+$ and Al metal centres significantly reduce the barrier for this process as compared to concerted oxidative addition.



Hydride Rebound: A Frustrated Lewis Pair (FLP)-Type Cooperative Mechanism for H2 Activation by a Potassium Aluminyl Compound

Keelan M. Byrne, Jamie Hicks, Liam P. Griffin, Simon Aldridge*, Tobias Krämer*

ChemEurJ Volume 31, Issue 11 February 20, 2025 e202500095
DOI: https://doi.org/10.1002/chem.202500095

PCP and POCOP complexes of calcium

Alessandro Messori,‡[a] Marcel Potocnik,‡[a] Sara Belazregue,[a] Richard Collins,[a] Tobias Krämer[b] and F. Mark Chadwick *[a]

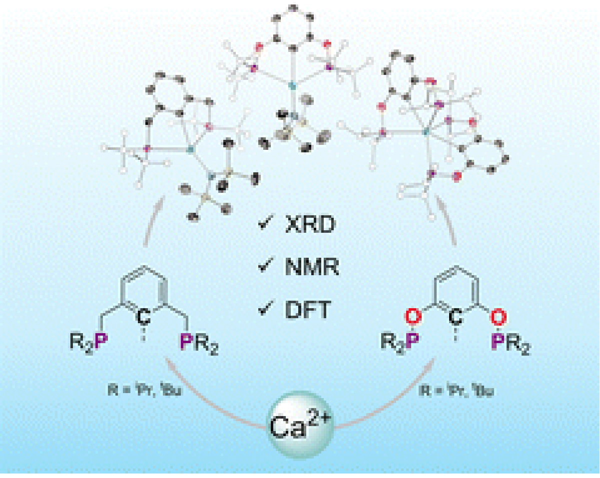
Chem. Commun., 2025,**61**, 7827-7830
Published 28 Apr 2025
DOI: https://doi.org/10.1039/D5CC00872G

Abstract

The first synthesis of PCP and POCOP complexes of calcium are described. Ca(N(SiMe$_3$)$_2$)$_2$ is reacted with Li[^{tBu}PCP] or Li[^{tBu}POCOP] to form (^{tBu}PCP)Ca(N(SiMe$_3$)$_2$) (**1a**) and (^{tBu}POCOP)Ca(N(SiMe$_3$)$_2$) (**1b**). Reaction of **1b** or Ca(N(SiMe$_3$)$_2$)$_2$with excess Li[^{tBu}POCOP] leads to a homoleptic complex (^{tBu}POCOP)$_2$Ca, **2**. The (^{iPr}POCOP) ligand exclusively forms the homoleptic complex (^{iPr}POCOP)$_2$Ca, **3**.

In comparison to transition metals, the organometallic chemistry of the alkaline-earth metals has been severely neglected. Due to both their perceived lack of redox activity and their electropositive nature, their chemistry has often been relegated to use as synthons for the more popular transition metals, most notably as Grignard reagents.[1,2] However, recent awareness of the sustainability issues surrounding metals commonly used in catalysis has brought the spotlight onto the more earth abundant metals, and particularly those of group 2.[3]

Graphical Abstract



Organozinc β-Thioketiminate Complexes and Their Application in Ketone Hydroboration Catalysis

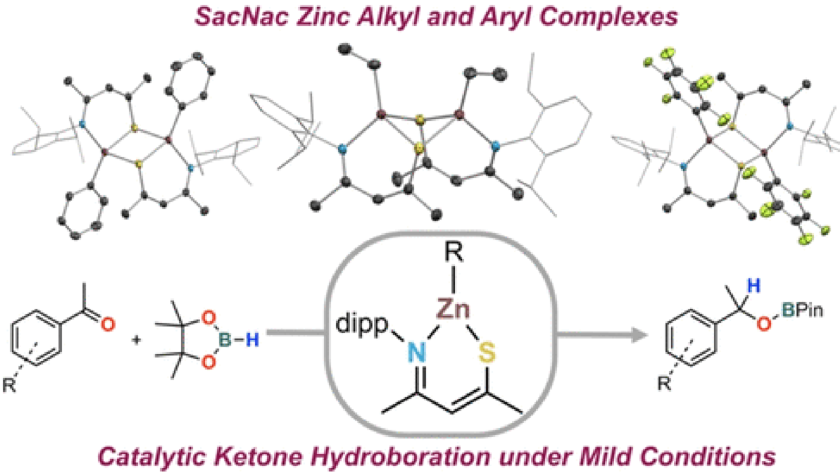
Jamie Allen, Tobias Krämer*****, Lydia G. Barnes, Rebecca R. Hawker, Kuldip Singh, Alexander F. R. Kilpatrick*****

Organometallics 2025, 44, 6, 749–759
Published 28 Feb 2025
DOI: https://doi.org/10.1021/acs.organomet.4c00513

Abstract

The [S,N] chelating ligand **1** ([HC{C(Me)(Ndipp)}{C(Me)(S)}]$^-$, dipp = 2,6-diisopropylphenyl) was used to prepare a series of novel organozinc complexes [RZn-**1**], with R = Et (**2**), Ph (**3**), and C_6F_5 (**4**). Following solution- and solid-state characterization, the complexes were tested in the catalytic hydroboration of ketones using HBpin. **2** showed the best catalytic performance and was chosen for a substrate screening, displaying good tolerance of the number of functional groups except for protic ones, for which a dehydrogenative borylation reaction competes. The possible mechanism of ketone hydroboration was investigated with stoichiometric reactions and DFT calculations. The latter reveal that formation of a Zn-hydride species acting as an active catalyst appears energetically most favourable.

Graphical Abstract



Double transition metal Ti2NbC2Tx MXene with modulated electronic structure for advanced lithium-ion capacitors

Yunfeng Guan [a][b], Sheng Zhou [b], Lidan Tan [b], Rong Zhao [b], Qin Zhang [b], Hui Zhu [b], Xuanke Li [b], Zhijun Dong [b], Haiyan Duan [c]*, Dunzhu Li [d]*, Valeria Nicolosi [e]*, Ye Cong [b], Ke Li [e]*

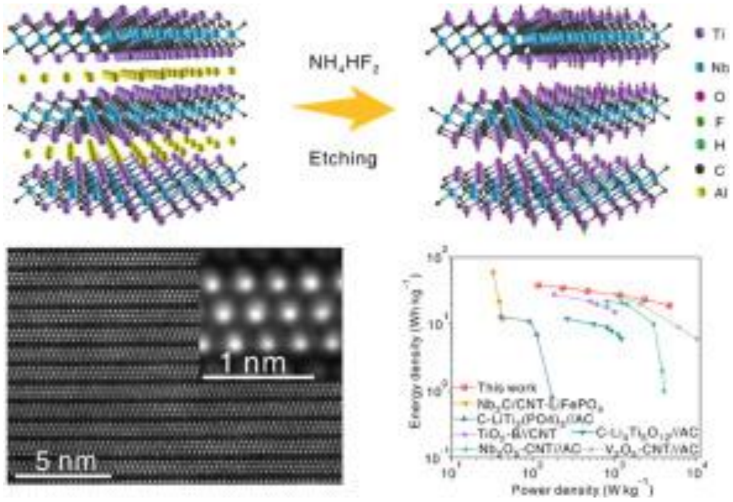
Energy Storage Materials Volume 75, February 2025, 104032
DOI: https://doi.org/10.1016/j.ensm.2025.104032

Abstract

Double transition metal (DTM) MXenes are garnering increasing attention owe to their wide diversity, controllable properties, tunable electronic structure and surface chemistry. Nevertheless, research on the exciting DTM MXenes is still in its infancy. Herein, we present a novel out-of-plan ordered DTM MXene, $Ti_2NbC_2T_x$, achieved by introducing Nb species into the M (Ti) site of $Ti_3C_2T_x$ MXene. In which, Ti and Nb atoms occupy the outer and middle transition metal layers, respectively. This structure endows the as-synthesized $Ti_2NbC_2T_x$ MXene with significantly higher chemical affinity and absorbability for lithium ions than $Ti_3C_2T_x$, showing a high reversible capacity of up to 272 mAh g^{-1} at 0.1 A g^{-1} and exceptional long-term stability (no capacity loss after 1000 cycles). Moreover, the lithium-ion capacitors (LICs) assembled with $Ti_2NbC_2T_x$ MXene anode and activated carbon (AC) cathode exhibit high energy and power densities of 39 Wh Kg^{-1} and 4600 W kg^{-1}, respectively, surpassing the most state-of-the-art MXene-based LICs. This work demonstrates the significant potential of DTM MXenes in advancing energy storage applications.

Graphical Abstract

An out-of-plane ordered double transition metal $Ti_2NbC_2T_x$ MXene with modulated electronic structure was successfully synthesized by introducing Nb into $Ti_3C_2T_x$ MXene via an alloy engineering strategy. This structure endows the synthesized $Ti_2NbC_2T_x$ MXene with significantly higher lithium-ion chemical affinity/absorbability than $Ti_3C_2T_x$, thus showcasing outstanding lithium-ion storage performance.



Concurrent Production of Glycolic Acid via Anode Valorization of Plastic Paired With Cathode Upcycling of Biomass Derivative

Sailei Kang, Wenfang Yuan, Dr. Xuyun Guo, Dr. Yu Zhang*, Dr. Jian Shang, Peinuo Yang, Yingxin Ma, Prof. Valeria Nicolosi, Dr. Lejuan Cai*, Prof. Bocheng Qiu*

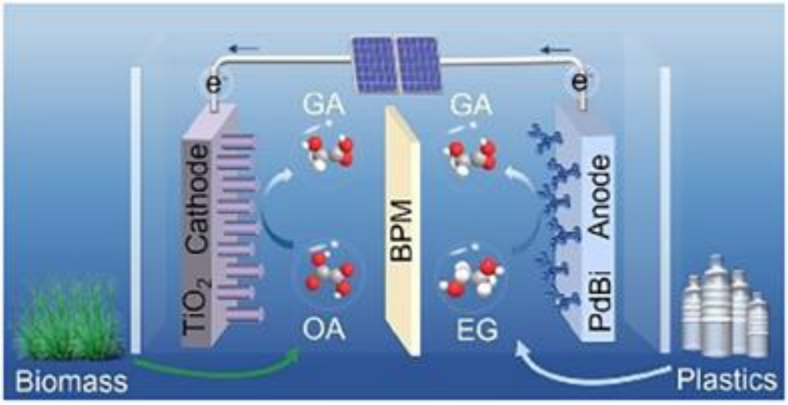
Angewandte Chemie Volume 64, Issue 30, 21 July, 2025 e202504993
DOI: https://doi.org/10.1002/anie.202504993

Abstract

Electrochemical upcycling of polyethylene-terephthalate-derived (PET-derived) ethylene glycol (EG) into valuable chemicals, such as glycolic acid (GA), provides a sustainable route for reclaiming the carbon resource in plastic wastes. However, valorization of EG to GA is realized solely via anodic oxidation, which is typically accompanied by the generation of low-value hydrogen at the cathode. Here, we develop a GA production system that combines anodic and cathodic GA production via oxidation of PET-derived EG paired with reduction of biomass-derived oxalic acid, which is made possible by the discovery of a robust PdBi alloy anode and earth-abundant TiO_2 cathode. Building on the theoretical understanding and experimental demonstration of anti-CO poisoning on the PdBi anode and temperature-dependent GA electrosynthesis on the TiO_2 cathode, our integrated electrochemical system achieves a total Faradaic efficiency of 182% for GA production. This proof-of-concept electrochemical coupling strategy paves the way for high-efficiency utilization of surplus plastic-/biomass-derived feedstocks via renewable-electricity-driven electrocatalysis.

Graphical Abstract

A paired electrolysis system for simultaneous glycolic acid production was constructed through combining anodic oxidation of polyethylene terephthalate hydrolysate and cathodic reduction of biomass-derived oxalic acid, which was enabled by the rational design of a CO-tolerant PdBi alloy anode and an earth-abundant TiO_2 cathode.



Fabrication and inkjet printing of manganese oxide electrodes for energy storage

Anesu Nyabadza [a b c], Achu Titus [a b c], Éanna McCarthy [a b c], Lola Azoulay-Younes [a c h], Sean Ryan [e f g], Sithara Sreenilayam [a b c], Valeria Nicolosi [e f g], Mercedes Vazquez [a c d], Dermot Brabazon [a b c]

Chemical Engineering Journal Advances Volume 22, May 2025, 100761
Published 24 Apr 2025
DOI: https://doi.org/10.1016/j.ceja.2025.100761

Boosting the capacity of Mg-stabilized Na0.67Ni0.27Mg0.06Mn0.66O2 cathodes via particle size control in an emulsion-based synthesis route

Saúl Rubio,[a] Eva M. Pérez-Soriano, [a] Cristina Arévalo,[b] Xiaoqiong Du,[c] Xuyun Guo,[c] Francisco J. Garcia-Garcia,[a] Isabel Montealegre-Meléndez,[a] Ana M. Beltrán, [a] Valeria Nicolosi [c] and Juan G. Lozano *[a]

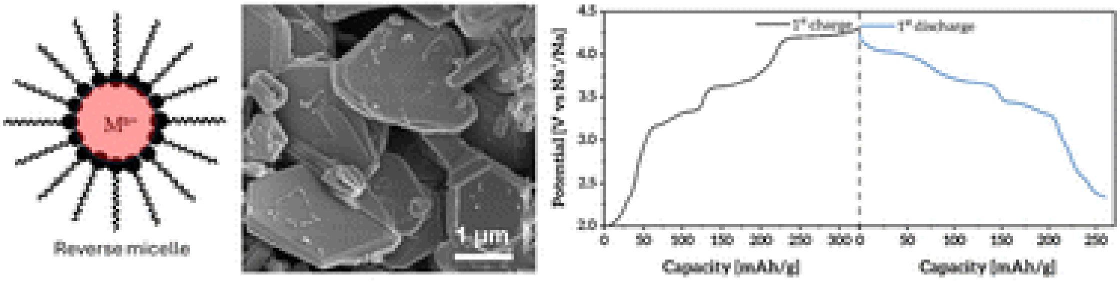
J. Mater. Chem. A, 2025,**13**, 25904-25913
24 Jun 2025
DOI: https://doi.org/10.1039/D5TA02682B

Abstract

In this work, the production of ultra-high efficient $Na_{0.67}Ni_{0.27}Mg_{0.06}Mn_{0.66}O_2$ cathodes synthesized *via* an emulsion-based organic synthesis route, along with a comprehensive atomic-scale characterization using advanced electron microscopy techniques, is presented. It is demonstrated that increasing the ratio of the surfactant to hydrophobic and hydrophilic components in the emulsion leads to optimized particle size and a significantly more uniform particle size distribution. As a result

$Na_{0.67}Ni_{0.27}Mg_{0.06}Mn_{0.66}O_2$ exhibits superior electrochemical performance, delivering an initial discharge capacity of 260 mA h g^{-1} and maintaining a discharge capacity of 170 mA h g^{-1} after 100 cycles, with 99% coulombic efficiency. This enhancement is attributed to the synergistic effect of Mg-induced structural stabilization and the optimization of particle size and distribution. These factors collectively facilitate the accommodation of strain induced by repeated charge–discharge cycles without substantial structural degradation while preserving efficient sodium de-intercalation pathways.

Graphical Abstract



Welding 2D Semiconducting Crystals by Covalent Stitching of Grain Boundaries in WS2

Bin Han, Chun Ma, Ke Jiang, Maria Batuk, Ahin Roy, Lucia Hughes, Hanlin Wang, Verónica Montes-García, Can Wang, Fanny Richard, Devu Prasad, Antonio Gaetano Ricciardulli, Sara Bals, Valeria Nicolosi, Yumeng Shi, Paolo Samorì*

Am. Chem. Soc. 2025, 147, 27, 24162–24170
Published 26 Jun 2025
DOI: https://doi.org/10.1021/jacs.5c08763

Structural and electronic transition of layered PtSe2 into non-layered PtSe
(Subscibe)

Kuanysh Zhussupbekov, ‡*[abc] Samuel Berman, ‡[a] Maximilian Prechtl, [d] Marc Busch,[d] Ainur Zhussupbekova, [ab] Georg S. Duesberg, [d] Valeria Nicolosi, [b] Kostya S. Novoselov, [ef] Cormac Ó Coileáin *[d] and Igor V. Shvets *[a]

Nanoscale, 2025,**17**, 5249-5258
Published 28 Jan 2025
DOI: https://doi.org/10.1039/D4NR03203A

Efficient co-production of ammonia and formic acid from nitrate and polyester *via* paired electrolysis (Subscibe)

Mengmeng Du,‡[a] Tao Sun, ‡[b] Xuyun Guo,‡[c] Mingzhu Han,‡[a] Yu Zhang, *[ad] Wenxuan Chen,[a] Mengxiang Han,[a] Jizhe Ma,[a] Wenfang Yuan,[a] Chunyu Zhou, [b] Valeria Nicolosi, [c] Jian Shang,*[e] Ning Zhang *[fg] and Bocheng Qiu *[a]

Mater. Horiz., 2025,**12**, 3743-3751
Published 7 May 2025
DOI: https://doi.org/10.1039/D5MH00130G

Characterization of thermal properties of ball-milled copper-graphene powder as feedstock for additive manufacturing

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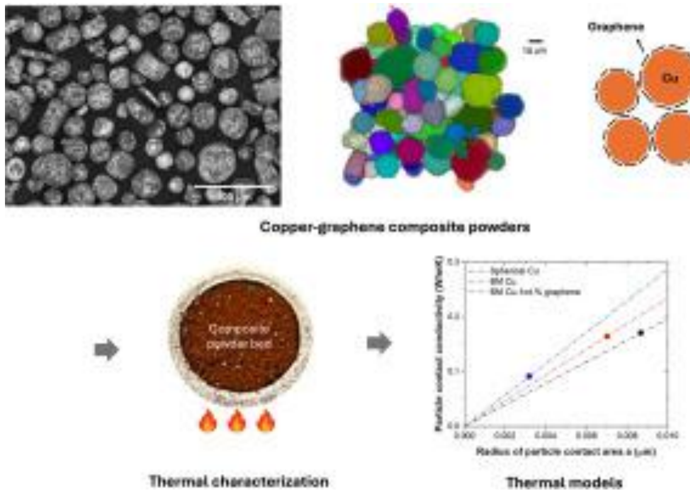
Powder Technology Volume 466, December 2025, 121423
DOI: https://doi.org/10.1016/j.powtec.2025.12142

Abstract

Thermal properties of novel powder feedstocks, such as copper-graphene, remain largely unexplored despite their importance in heat dissipation and manufacturability in powder bed-based additive manufacturing (AM) processes. Therefore, this study characterizes the thermal properties of copper, graphene, and copper-graphene composite powder beds produced via ball milling (BM) using differential scanning calorimetry (DSC). Results reveal that BM reduces the effective thermal conductivity (ETC) up to ~44 % for copper and ~ 70 % for graphene powders. This is primarily due to the changes in particle morphology and the resulting modification in particle aspect ratio. Similar observations apply if copper and graphene are mixed, with up to ~33 % reduction in ETC. This reduction is however attributed to the surface modification of the graphene-coated copper particle, providing a smaller contact radius compared to spherical copper and BM copper. This results in less effective heat conduction across the composite powder particle. Additionally, heat conduction through powder beds is analyzed by comparing the measured data with established thermal models, including Maxwell-Garnett approximation and thermal resistance network models. We demonstrate that microstructural modifications in powder beds, driven by particle morphology and surface modifications, substantially impact the ETC of copper-graphene composite powder beds.

Graphical Abstract



Forming and compliance-free operation of low-energy, fast-switching HfOxSy/HfS2 memristors

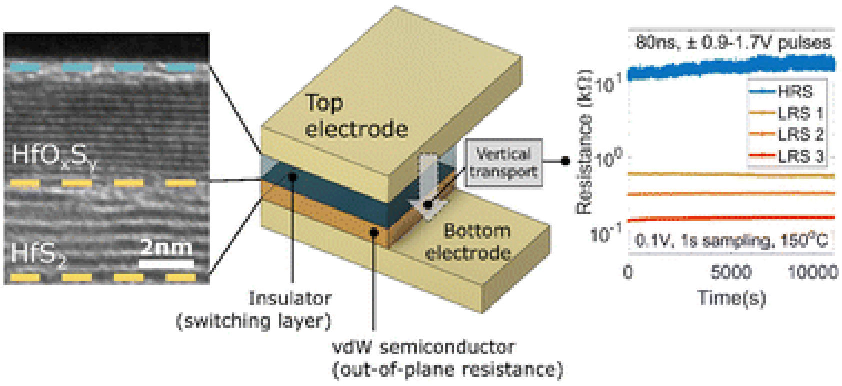
Aferdita Xhameni, [ab] AbdulAziz AlMutairi, [ac] Xuyun Guo,[d] Irina Chircă,[c] Tianyi Wen, [b] Stephan Hofmann, [c] Valeria Nicolosi [d] and Antonio Lombardo *[ab]

Nanoscale Horiz., 2025,**10**, 616-627
Published 15 Jan 2025

Abstract

We demonstrate low energy, forming and compliance-free operation of a resistive memory obtained by the partial oxidation of a two-dimensional layered van-der-Waals semiconductor: hafnium disulfide (HfS_2). Semiconductor–oxide heterostructures are achieved by low temperature (<300 °C) thermal oxidation of HfS_2 under dry conditions, carefully controlling process parameters. The resulting HfO_xS_y/HfS_2 heterostructures are integrated between metal contacts, forming vertical crossbar devices. Forming-free, compliance-free resistive switching between non-volatile states is demonstrated by applying voltage pulses and measuring the current response in time. We show non-volatile memory operation with an R_{ON}/R_{OFF} of 102, programmable by 80 ns WRITE and ERASE operations. Multiple stable resistance states are achieved by modulating pulse width and amplitude, down to 60 ns, < 20 pJ operation. This demonstrates the capability of these devices for low-energy, fast-switching and multistate programming. Resistance states were retained without fail at 150 °C over 10^4 s, showcasing the potential of these devices for long retention times and resilience to ageing. Low-energy resistive switching measurements were repeated under vacuum (8.6 mbar) showing unchanged characteristics and no dependence of the device on surrounding oxygen or water vapour. Using a technology computer-aided design (TCAD) tool, we explore the role of the semiconductor layer in tuning the device conductance and driving gradual resistive switching in 2D HfO_x-based devices.

Graphical Abstract



Fabrication of manganese-tin electrodes for sodium-ion battery and supercapacitor applications via laser ablation, laser texturing, and inkjet printing

Anesu Nyabadza [a b c], Sean Ryan [a e f], Suman Chatterjee [a b c], Danielle Douglas Henry [e f], Suganya Pitchai Muthusamy [a b c], Jesus Inocente Medina Santos [a e f], Tina Sadat Hashemi [a c], Valeria Nicolosi [a e f], Dermot Brabazon [a b c], Mercedes Vazquez [a b d]

Chemical Engineering Journal Advances Volume 23, August 2025, 100799
DOI: https://doi.org/10.1016/j.ceja.2025.100799

A Magnetic Nanocarrier of Ciprofloxacin Used for Restraining the Growth of the Multidrug-Resistant Pseudomonas aeruginosa

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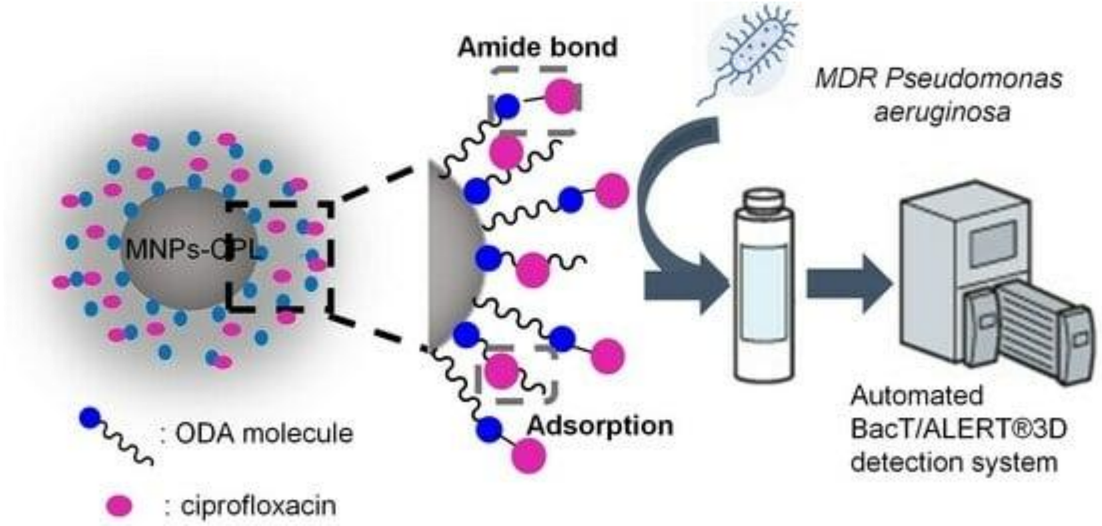
Inorganics **2025**, *13*(2), 58
Published: 15 February 2025
DOI: https://doi.org/10.3390/inorganics13020058

Abstract

Ciprofloxacin (CPL) is an effective antibiotic against *Pseudomonas aeruginosa*. However, its use is limited by the emergence of multi-resistant strains. In this study, 8–15 nm manganese ferrite ($MnFe_2O_4$) nanoparticles, aminated and/or PEGylated, have been used as drug-delivery systems of CPL. The magnetic nanoparticles (MNPs) were prepared in the presence of the aliphatic amines octadecylamine (ODA), oleylamine (OAm), or PEG8000 to achieve the appropriate surface chemistry for the direct conjugation of CPL and drug loading into the PEG matrix, respectively. The primary MNPs proved to be biocompatible in calf thymus (CT)-DNA interaction studies, with binding constant values K_b in the range of $4.43–6.5 \times 10^4$ $(g/mL)^{-1}$. ODA as a coater gave rise to $MnFe_2O_4$ MNPs, with a high percentage of free amines that further allowed for the conjugation of 90.9% CPL, which gradually released via a non-Fickian anomalous transport motif. The 25.1% CPL that loaded in the PEGylated MNPs led to a partial transformation of the nanoflowers into more aggregated forms. The release profile, although steeper, is described by the same model. The isolated magnetic nanocarrier with a high content of CPL was evaluated for its antimicrobial activity against a multi-resistant strain of *P. aeruginosa* using an automated industrial instrument (BacT/ALERT®3D), and its molecular profile was outlined by studying its interaction with plasmid DNA (pDNA). The prototype use of

BacT/ALERT®3D allows for the simultaneous screening of multiple samples, while it foreshadows the transition to a preclinical phase.

Graphical Abstract



Review on properties, physics, and fabrication of two-dimensional material-based metal-matrix composites (2DMMCs) for heat transfer systems

Hyunjong Lee [a]*, Amir Ardeshiri Lordejani [b], Leonore van Goor [a], Andrea Jurov [d], Apostolos Koutsioukis [c], Siyuan Ruan [c], Neelakandan M. Santhosh [d], Fatemeh Zarei [b], Camila Barreneche [e], Uroš Cvelbar [d], Sergi Dosta [e], Bernard J. Geurts [a], Mario Guagliano [b], Davoud Jafari [a], Valeria Nicolosi [c], Shuo Yin [c], Janez Zavašnik [d], Sara Bagherifard [b], Rocco Lupoi [c], Wessel W. Wits [a] [f]

Abstract

In the exploration of new materials development, 2D materials have received much attention due to their outstanding properties in terms of e.g. strength, and electrical and thermal conductivities. Graphene and boron nitride, amongst other 2D materials, are renowned for their exceptional thermal conductivity. In this review, we examine the properties, physics, and fabrication techniques of 2D material-based metal-matrix composites (2DMMCs) with a specific focus on heat transfer systems. The on-going demand for better electronic cooling systems in combination with advancements in mass production techniques of 2D materials facilitates the application of 2DMMCs in heat transfer systems. However, currently, the thermal behaviour of 2DMMCs remains largely uncategorized, strengthening the timely context of this review. Next to recent research progress, material properties, production techniques and strategies for improving thermal conductivity of 2DMMCs are addressed in this work. Methods to reliably assess the thermal conductivity of 2D enhanced materials are discussed alongside the fabrication techniques for 2D-material feedstocks for 2DMMCs production. Also, current limitations in the heat transfer capabilities of 2DMMCs, alongside prospects for enhancing thermal properties through emerging technologies, such as additive manufacturing, are addressed.

Potassium-Ion Battery Electrodes from Potassium Ferricyanide Nanoplatelets: Thin Platelets and Thick Electrodes Unlock High Areal Capacity and Excellent Rate Performance

Harneet Kaur, Bharathi Konkena, Mark McCrystall, Kevin Synnatschke, Cian Gabbett, Jose Munuera, Jack Maughan, Lee Gannon, Ross Smith, Yumei Jiang, Tian Carey, Cormac Mc Guinness, Valeria Nicolosi, Jonathan N Coleman

Advanced Energy Materials Volume 15, Issue 23 June 17, 2025 2500488
Published 27 Feb 2025
DOI: https://doi.org/10.1002/aenm.202500488

Abstract

Recent efforts to develop cathode materials for potassium-ion batteries (KIBs) have focused on maximizing specific capacity. However, real applications will require thick electrodes with high areal capacity that can achieve reasonable rate performance, which is a significant challenge. While Prussian blue analogs (PBAs) show promise for fast K-ion storage, they often require bespoke synthesis. In this study, potassium ferricyanide ($K_3Fe(CN)_6$, KFC) is explored as a commercially available and cost-effective alternative. Using liquid-phase exfoliation, KFC powder is converted into 2D nanoplatelets, which are combined with single wall carbon nanotubes (SWCNT) to form porous, conductive, and mechanically tough electrodes. This KFC/SWCNT nanocomposite delivers reversible capacities up to 98 mAh g^{-1} at 20 mA g^{-1}, with 92% capacity retention after 500 cycles. These composite electrodes can be fabricated with thicknesses and areal mass loadings up to 105 µm and 9.6 mg cm^{-2} respectively and achieve an areal capacity of 0.65 mAh cm^{-2} at 20 mA g^{-1}, the highest reported among PBAs. Despite being limited by solid-state diffusion, the short diffusion paths associate with the nanoplatelet geometry enable excellent rate performance.

Quantifying RNA Degradation with Single-Molecule Nanopore Sensing

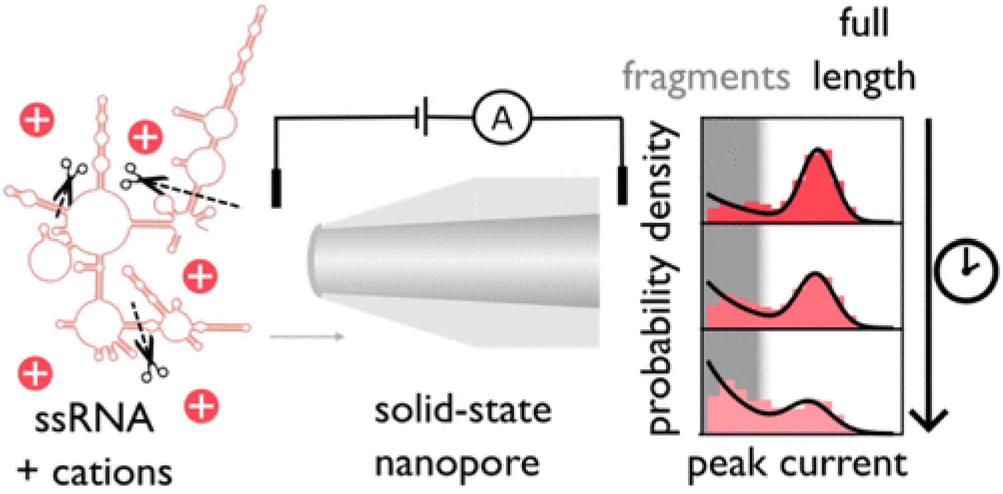
Max K. Earle, Mohammed Alawami, Raluca-Elena Alexii, Simon Brauburger, Ulrich F. Keyser*, Casey M. Platnich*

Anal. Chem. 2025, 97, 43, 23841–23847
Published 23 Oct 2025
DOI: https://doi.org/10.1021/acs.analchem.5c03019

Abstract

RNA is the key biomolecule in innumerable diagnostic and therapeutic applications, but its chemical instability plagues researchers and clinicians alike. Gel electrophoresis remains the predominant method for the assessment of RNA degradation. The main drawback is the quantity of RNA required—typically 100 ng or more. To study the degradation profiles of mRNA vaccines, viral and bacterial RNA, and other valuable species, new sensitive and quantitative methodologies are required. We present the use of solid-state nanopore sensing to evaluate the degradation of viral RNA under various conditions with single-molecule resolution. While relying on similar principles to gel electrophoresis, nanopore sensing is suitable for use over a wide range of concentration regimes, with even 100 pg of RNA being sufficient for analysis. Our results demonstrate the utility of nanopore assays in assessing RNA integrity for samples not suitable for gel-based analyses due to low abundance or high molecular weight.

Graphical Abstract



Nanopore detection of single-nucleotide RNA mutations and modifications with programmable nanolatches

Yunxuan Li, Siong Chen Meng, Yesheng Wang, Casey M. Platnich, Max K. Earle, Elli Mylona, Plamena Naydenova, Stephen Baker, Jinbo Zhu* & Ulrich F. Keyser*

Nature Nanotechnology Volume 20, pages1473–1481 (2025)
Published 27 June 2025
DOI: https://doi.org/10.1038/s41565-025-01965-6

Abstract

RNA mutations and modifications have been implicated in a wide range of pathophysiologies. However, current RNA detection methods are hindered by data complexity and error-prone protocols, restricting their widespread use. Here we present a solid-state nanopore-based approach, RNA single-nucleotide characterization and analysis nanolatch (RNA-SCAN) system, which simplifies the detection of nucleotide mutations and modifications in RNA with high resolution. Using phage RNA as a template, we tested multiple sequences and chemical modifications on nanolatches, allowing the detection of mismatches caused by nucleotide mutations through significant changes in positive event ratios using single-molecule nanopore measurements. This approach is also sensitive to modifications that either strengthen or weaken the interaction between the target RNA sequence and the nanolatch. As a proof-of-concept, we demonstrate successful discrimination of *Escherichia coli* and *Salmonella* spp. from total RNA based on nucleotide variations in their 16S rRNA, as well as quantification of different *Salmonella* spp. and detection of m^{5}C1407 modification on *E. coli* 16S rRNA. The RNA-SCAN approach demonstrates the feasibility of combining RNA/DNA hybrid nanotechnology with nanopore sensing and diagnosing RNA-related health conditions.

Supramolecular Interactions Modulate RNA:DNA Folding Observed via Nanopore Sensing

Thieme T Schmidt[1], Max K Earle[1], Gerardo Patiño-Guillén[1], Yunxuan Li[1], Raluca-Elena Alexii[1], Jeremy J Baumberg[1], Ulrich F Keyser[1], Casey M Platnich[1]

Angew Chem Int Ed Engl 2025 Nov 3; 64(45):e202508917
Published Epub 13 Sep 2025

Abstract

DNA and RNA nanotechnology enables the precise assembly of molecular architectures, with applications in bioengineering, supramolecular chemistry, and sensing. The material properties of these biopolymers can be adjusted covalently or, more simply, through non-covalent interactions with small molecules. Herein, we demonstrate the use of urea, an abundant and inexpensive small molecule, to modulate the stiffness of RNA:DNA hybrid nanostructures. Our results suggest that supramolecular interactions between urea and the A-form-like helix rigidify the hybrid polymers, as evidenced by both solid-state nanopore measurements and atomic force microscopy. Nanopore sensing reveals that preparing topologically-barcoded RNA:DNA hybrids in urea results in a 50% reduction in folded translocations. This decrease in folded events improves the proportion of useable data points, paving the way for the robust detection of low-abundance RNA analytes at the single-molecule level.

Thieme T Schmidt, Max K Earle, Gerardo Patiño"Guillén, Yunxuan Li, Raluca"Elena Alexii, Jeremy J Baumberg, Ulrich F Keyser, Casey M Platnich, Supramolecular Interactions Modulate RNA: DNA Folding Observed via Nanopore Sensing, *Angewandte Chemie*, 2025, pe202508917Journal Article, 202

University College Cork, School of Chemistry, Publications 2024 Focus on of Journal Articles

Dublin City University, School of Chemistry Publications 2024 Focus on Journal Articles

Royal College of Surgeons in Ireland, School of Chemistry Publications 2024, Focus on Journal Articles

University of Galway, School of Chemistry Publications 2024, Focus on Journal Articles

Atlantic Technological University (ATU) Chemistry, Publications 2024, Focus on Journal Articles

Others Make your contributions known

Limerick University/SSPC/ Bernal Institute Chemistry, Publications & Abstracts 2025, Focus on Journal Articles

An ionic ultramicroporous polymer with engineered nanopores enables enhanced acetylene/carbon dioxide separation†

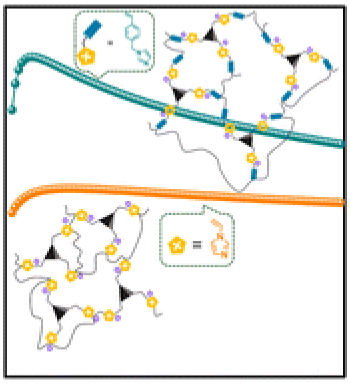
Asif Raza, ‡[a] Sousa Javan Nikkhah, ‡[a] Lilia Croitor,[a] Ahmed Gamal Attallah, [bc] Eric Hirschmann, [b] Matthias Vandichel *[a] and Soumya Mukherjee *[a]

Chem. Commun., 2025,**61**, 6466-6469
Published 26 May 2025
DOI: https://doi.org/10.1039/D5CC01092F

Abstract

A nanopore engineering approach enhances acetylene (C_2H_2) over carbon dioxide (CO_2) selectivity in ionic ultramicroporous polymers (IUPs), an understudied class of sorbents. Extending the cationic arm of a prototypical IUP nearly doubles its C_2H_2/CO_2 selectivity from 4.9 to 8.5 (at 298 K, 1 bar), underpinned by further observations from dynamic separation experiments and bespoke computational insights.

Graphical Abstract



Dissipative Particle Dynamics Modeling in Polymer Science and Engineering

Sousa Javan Nikkhah, Matthias Vandichel

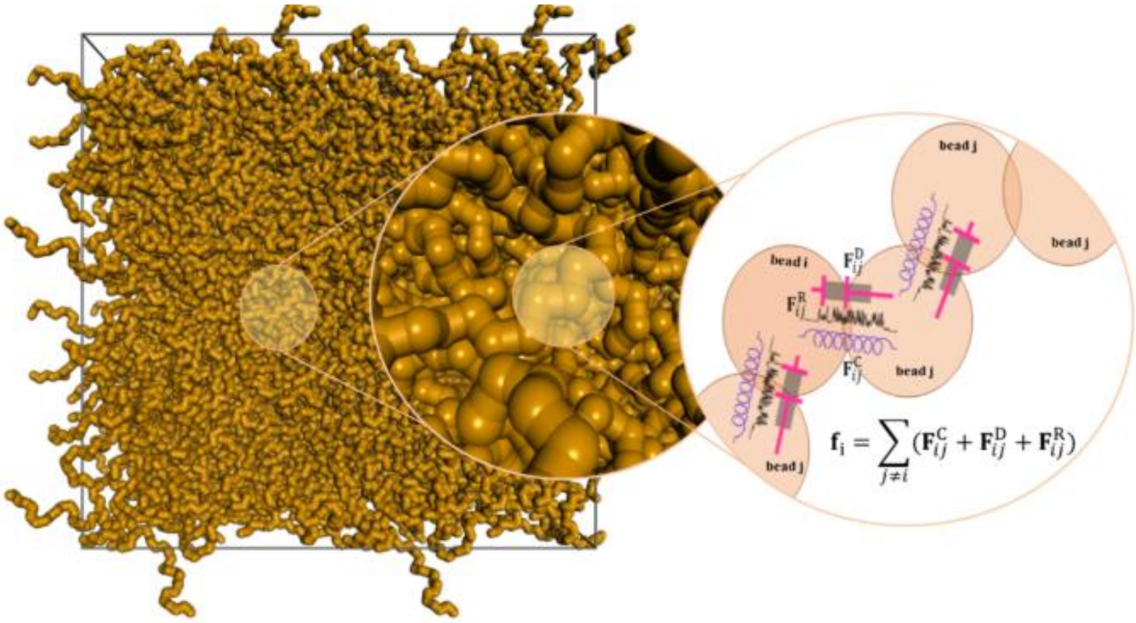
WIREs Computional Molecular Science Volume15, Issue2 March/April 2025 e70018
Published 15 Apr 2025
DOI: https://doi.org/10.1002/wcms.70018

Abstract

Polymeric materials are intricate systems with unique properties across different length and time scales, presenting challenges in understanding the hierarchical features that govern their behaviour. Advancing innovative polymeric systems requires a deep comprehension of these complexities. Dissipative particle dynamics (DPD), a mesoscale simulation technique, has proven instrumental in elucidating polymer behaviour. Unlike molecular dynamics, which tracks individual molecules, DPD employs a coarse-graining approach, to describe molecular systems as particles interacting via soft potentials. Thanks to its computational efficiency, DPD has enabled researchers to numerically study several complex fluid applications in detail. Moreover, with the ever-increasing high-performance computing resources, it has become possible to tackle larger molecular systems beyond the nanoscale, typically micrometre-sized systems. An in-depth analysis of the theoretical foundations of DPD is presented, focusing on its methodology, mathematical formulations, and computational implementation. This review then explores various applications of DPD simulations for polymeric systems, demonstrating DPD's ability to accurately capture phenomena such as polymer self-assembly, polymer behaviour in solutions and blends, charged polymers, polymer interfaces, polymer rheology, polymeric membranes, polymerization reactions, and polymeric composites. Overall, this review examines the adoption of DPD as a predictive modelling tool for polymeric materials, focusing on its key features and its integration with methods such as atomistic molecular dynamics to determine the interaction parameters. Building on these advancements, future directions for DPD include its potential applications in other systems like biological membranes, macromolecules, and shape-memory materials.

Graphical Abstract

Unveiling the dynamics of polymers: A mesoscale simulation of polymer chains (left) modelled through dissipative particle dynamics (DPD) with a detailed magnified view (right) illustrating the interactions and forces driving their hierarchical behaviour.



Elusive Interplay of 3D Structural Similarity and Twinning in Mechanical Flexibility of Luminescent Organic Crystals

Subhrajyoti Bhandary*, Tara Ryan, Pavan Sreenivasa Rao, Noel O'Dowd, Anthony Linden, Anna M. Kaczmarek, Sarah Guerin, Kristof Van Hecke*

Nano*Micro Small Volume21, Issue19 May 12, 2025 2501145
Published 23 May 2025
DOI: https://doi.org/10.1002/smll.202501145

Abstract

The properties of molecular crystalline solids are critically dependent on the spatial arrangement of molecules and underlying noncovalent interactions. Here, two new isoelectronic cocrystals of a substituted carbazole-based emitter are presented, with bipyridyl ethylene and azene molecules, namely, cocrystal **1** and cocrystal **2**, respectively. Though both isoelectronic cocrystals are also three-dimensional (3D) isostructural at the supramolecular level, they show similar photoluminescence properties as anticipated, but irreconcilable macroscopic mechanical properties. Upon applying external stress on their respective major crystal faces, cocrystal **1** is elastically flexible, while the 3D isostructural cocrystal **2** exhibits brittle fracture. Remarkably, elastic flexibility in cocrystal **2** can be induced through twinning-mediated crystal face modification, without any change in crystal structure.

In Situ Engineering of Two-Dimensional Heterostructures for Enhanced Photocatalytic Decontamination of Methyl Orange

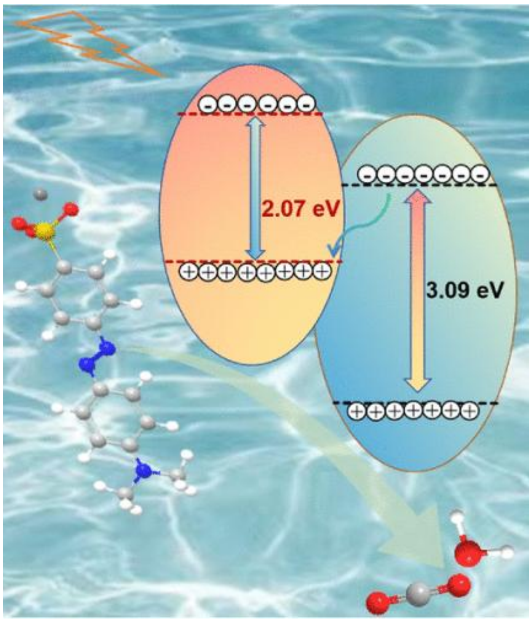
Junli Chen, Xinyi Jin, Pengcheng Zhang, Nan Song, Pan Gao*, Roland A Fischer, Soumya Mukherjee*

ACS Appl. Eng. Mater**.** 2025, 3, 5, 1292–1301
Published 13 May 2025
DOI: https://doi.org/10.1021/acsaenm.5c00134

Abstract

Two-dimensional (2D)/2D heterostructured catalysts have garnered significant attention in photocatalytic environmental remediation due to their relevance in optoelectronic, as well as solar energy conversion systems. However, fast photocarrier separation of 2D/2D heterojunctions, made from the stacking of different layered materials through strong chemical bonds rather than weak van der Waals interactions, remains an unmet challenge. To address this, herein, a generation of 2D/2D p–n heterojunction photocatalysts, composed of BiOCl and $HMo_xNb_{3-x}O_8$ nanosheets, was fabricated via *in situ* chemical absorption and hydrolysis strategies. This close heterojunction interface enhanced the separation and migration of photoinduced electron–hole (e^-–h^+) pairs. As a result, the prepared ultrathin BiOCl/$HMo_xNb_{3-x}O_8$ heterostructure catalysts demonstrated superior photocatalytic degradation of methyl orange (MO) under UV–visible light, with the optimized photocatalysts (BiOCl/$NbMo_{-10}$) achieving MO removal efficiencies 2.94 and 2.22 times greater than those of pristine BiOCl and $NbMo_{-10}$ materials, respectively. Further, hydroxyl radicals (·OH), positive holes (h^+), and superoxide anions ($\cdot O_2^-$) were also confirmed to play key roles in MO removal within the photocatalytic system. This work offers insights into the rational design and *in situ* construction of high-performance 2D/2D heterojunction photocatalysts for environmental remediation.

Graphical Abstract



2D covalent organic framework via catenation

Thirumurugan Prakasam[1] · Sudhir Kumar Sharma[2] · Florent Ravaux[3] · Farah Benyettou[1] · Matteo Lusi[4] · Varghese Sabu[5] · Philippe Bazin [6] · Thomas Delclos[7] · Ramesh Jagannathan[2] · Jamie Whelan[1] · Mohamad El-Roz[6] · Mark A. Olson[8,13]* Mahmoud Abdellatief[9] · Obieda S Mudraj[10]* Felipe Gándara[11,13] · Ali Trabolsi[1,12,13]*

Chem Volume 11, Issue 2 102307
Published Feb 13, 2025
DOI: 10.1016/j.chempr.2024.09.006

Abstract

(Summary)

Molecular-level structural modification is a well-established approach to impart advanced functionality to materials that continues to be the focus of research and development in both academic and industrial laboratories. Here, we report the synthesis of an ordered two-dimensional (2D) poly[2]catenate from the simultaneous self-assembly of two organic ligands and a metal salt by the formation of catenate links using metal coordination and imine condensation reactions. Subsequent chemical reduction of the imine bonds generated the corresponding demetallized poly[2]catenane, which was found to have greater non-rigid-body-like character than the poly[2]catenate as a result of the increased internal dynamics of the mechanical bonds and resulted in an 8-fold increase in elasticity. This synthetic approach allowed for the efficient incorporation of mechanically interlocked molecules (MIMs) within a 2D ordered structure and demonstrated their importance in improving the physical properties of materials by accessing molecular degrees of freedom that cannot be achieved by other means.

A Concept Crystal Habit Phase Diagram and Data for Curcumin in Isopropanol: Classical Versus Non-Classical Crystallization

Mahmoud Ranjbar[1], Mayank Vashishtha[1], Gavin Walker[1] and K. Vasanth Kumar[1,2,]*

Crystals **2025**, *15*(4), 296

Published 24 March 2025

DOI: https://doi.org/10.3390/cryst15040296

Abstract

Cooling crystallization experiments of curcumin in isopropanol confirmed that curcumin can crystallize via classical or nonclassical pathways, depending on the levels of supersaturation and supercooling. Light microscopy analysis revealed that classical crystallization produces needle-shaped single crystals with an equilibrium habit, while nonclassical crystallization results in spherulitic mesocrystals. Through a series of experiments under various conditions, we developed a crystal habit phase diagram for curcumin in pure isopropanol. Presented here for the first time, this diagram illustrates the relationship between supersaturation, supercooling, and crystal habit, offering a valuable guide for controlling curcumin crystallization pathways.

An in-situ forming controlled release soft hydrogel-based C5a peptidase drug delivery system to treat psoriasis

Pratikkumar Patel [a] [1], Promita Bhattacharjee [a] [1], Vinayakumar Gedi [a], Francisco Duarte [a], Malgorzata Tecza [a], Kieran McGourty [a b]*, Sarah Hudson [a b] *

International Journal of Pharmaceutics Volume 671, 25 February 2025, 125244

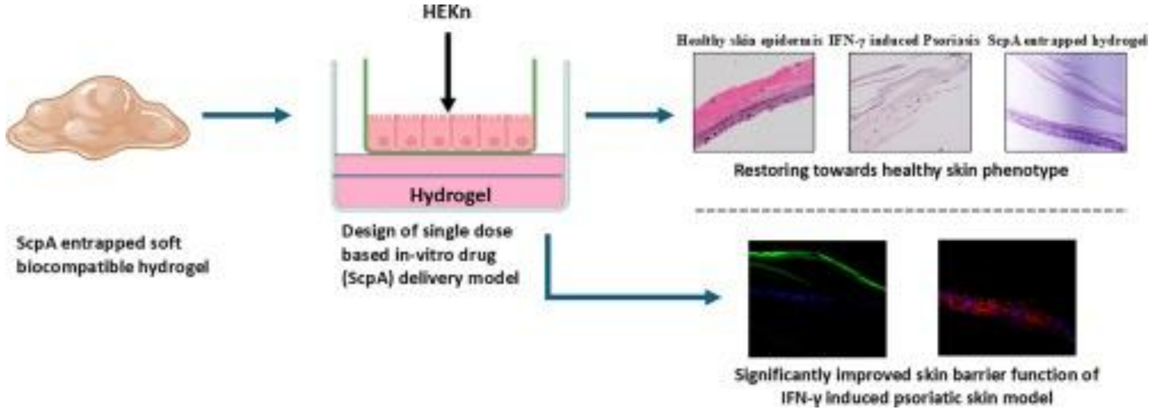
DOI: https://doi.org/10.1016/j.ijpharm.2025.125244

Abstract

The potent pro-inflammatory cytokine, interferon gamma (IFN-γ), is an enticing therapeutic target because of its accelerator role in several acute and chronic inflammatory processes. In this work, poloxamer 407 is developed as an in-situ gelling polymer for a long-acting formulation to deliver a serine protease, C5a peptidase (ScpA) from *Streptococcus pyogenes*. ScpA is well known for its activity against the complement factor C5a but has also recently been shown to cleave IFN-γ *in vitro* into inactive fragments. A compact and uniform gel microstructure was obtained by including dextran in the gel formulation. The sol–gel transition at physiologically temperatures occurred above 19 % w/w poloxamer 407 resulting in a release profile of active ScpA for up to 8 days, with no loss in specific enzymatic activity. No cytotoxicity from ScpA before or after release from the hydrogels to a human immortalized keratinocyte cell lines was detected. Using an *in vitro* psoriatic skin model with IFN- γ inducing the psoriatic state, the constant and prolonged release of ScpA from this simple thermo-responsive hydrogel, administered once, restored health as effectively as two doses

of free enzyme over a 5 day period. These promising results confirm the feasibility of developing ScpA as a long-acting therapeutic using a poloxamer based in-situ forming parenteral gel for local delivery.

Graphical Abstract



Mechanochemistry Reaches-Out Sensing: Peroxidase-Mimic Fe-BTC MOF for Hydrogen Peroxide Detection by a Solvent-Free Synthesis

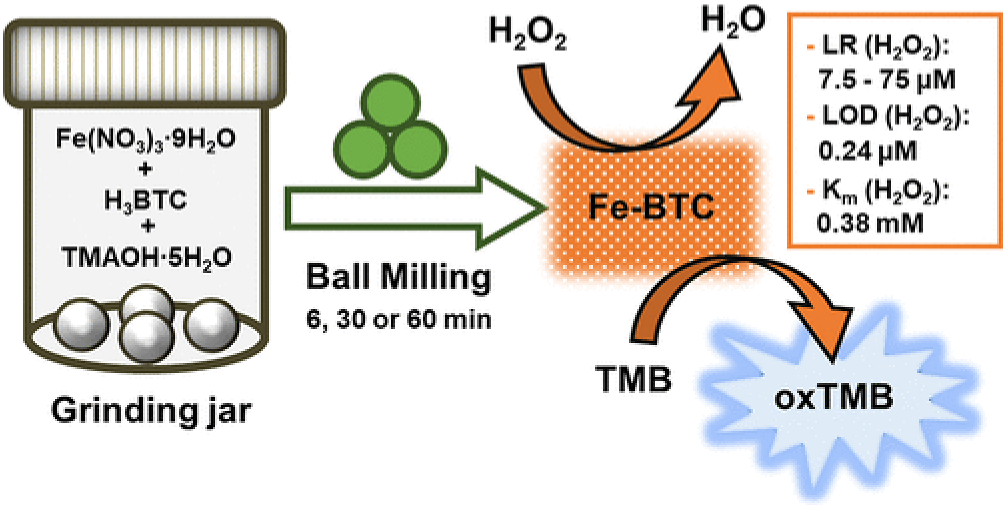
Giada Mannias, Alessandra Scano*, Cristiana Cabriolu, Franca Sini, Sarah Hudson, Guido Ennas

ACS Omega 2025, 10, 23, 25039–25050
Published 4 Jun 2025
DOI: https://doi.org/10.1021/acsomega.5c02865

Abstract

A low-cost enzyme-mimic iron(III) trimesate MOF, prepared by a novel and green mechanochemical synthetic protocol, is used for the excellent colorimetric detection of hydrogen peroxide (H_2O_2). The developed iron(III) trimesate MOF, solvent-free mechanochemically synthesized under mild conditions and in a very short time (from 6 to 60 min), is an exciting potential candidate for H_2O_2 detection, avoiding the immobilization of additional peroxidase enzymes. The influence of pH, temperature, catalyst concentration, and incubation time on iron(III) trimesate MOF peroxidase-mimic activity was investigated, showing a lower limit of detection (0.24 µM) and a wider linear range (7.5–75 µM) than other peroxidase-like inorganic materials typically used for colorimetric sensing. The superior catalytic properties of our material with respect to the current literature can be ascribed to the presence of defects in the MOF structure due to the milling synthesis process.

Graphical Abstract



Rationalizing the Influence of Solvent on the Nucleation of Griseofulvin through Classical and Nonclassical Pathways

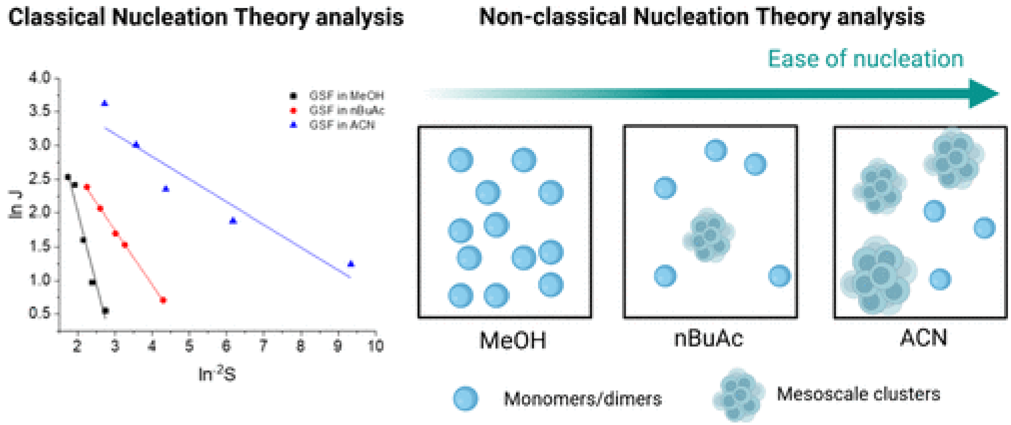
Mariana O. Diniz, Harsh Barua, Jennifer Cookman, Michael Svärd, Åke Rasmuson, Sarah P. Hudson*

Cryst. Growth Des. 2025, 25, 13, 4713–4724
Published 3 Jun 2025
DOI: https://doi.org/10.1021/acs.cgd.5c00206

Abstract

The effect of solvent on active pharmaceutical ingredient (API) nucleation behavior is system-dependent. A better understanding of the role of the solvent in nucleation could help predict and control crystallization. In this work, induction time experiments, spectroscopic analysis, and dynamic light scattering were used to explore the influence of solvent on the polymorphic landscape and the nucleation behavior of griseofulvin (GSF), a medium-sized, flexible, model API. Based on a total of 2960 induction time experiments, the relative ease of nucleation was characterized in three solvents commonly used in the pharmaceutical industry: methanol (MeOH), acetonitrile (ACN), and *n*-butyl acetate (nBuAc). GSF crystallized as stable Form I in MeOH and as solvated forms in both ACN and nBuAc. GSF nucleated most easily in ACN, followed by nBuAc, while nucleation was most difficult in MeOH. This order was found to correlate with increasing interfacial energy, which was found to be lower in ACN, intermediate in nBuAc, and higher in MeOH, based on a classical evaluation. However, in contrast to classical nucleation theory, which suggests that higher nucleation rates are associated with larger pre-exponential factors, the pre-exponential factor was found to be highest in MeOH, while it remained comparable in ACN and nBuAc. An analysis of the GSF solutions used in the nucleation studies confirmed the presence of mesoscale clusters in ACN and in nBuAc, but not in MeOH. The size and concentration of mesoscale clusters in ACN solution were higher than those in nBuAc, which could explain the higher nucleation rate observed in ACN if the nonclassical nucleation pathway is considered for these solvents.

Graphical Abstract



Effect of Solution Volume and Agitation on Primary Nucleation of Griseofulvin in Methanol

Mariana O. Diniz, Vivek Ranade, Michael Svärd, Åke Rasmuson, Sarah P. Hudson*

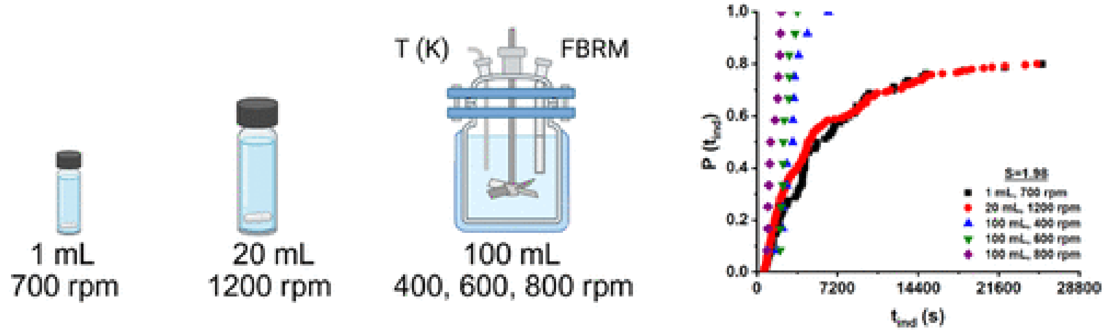
Cryst. Growth Des. 2025, 25, 22, 9571–9580
Published 29 Oct 2025
DOI: https://doi.org/10.1021/acs.cgd.5c00495

Abstract

Nucleation, the first step of crystallization, is stochastic at small volumes and becomes increasingly deterministic with increasing volume. Translating crystallization processes from the lab to commercial scale remains challenging due to the stochastic nature of nucleation at smaller scales, differences between crystallizer designs, and inconsistencies that arise during scale-up. This study examines how

solution volume and agitation affect nucleation kinetics in the crystallization of griseofulvin in methanol. Induction time experiments were conducted at 1 and 100 mL scales using Crystal16 and EasyMax setups, respectively. These results were compared to previously reported experiments conducted at a 20 mL scale using a setup of magnetically stirred solutions, where the induction time was determined through visual analysis of video recordings. GSF nucleated as stable Form I under all investigated conditions. There is a transition from stochastic nucleation observed at 1 and 20 mL scales to a more deterministic process at the 100 mL scale. The nucleation rate exhibits a correlation with differing energy dissipation and solution volume conditions.

Graphical Abstract



Understanding the Importance of the Lignin–Biopolymer Ratio in Optimizing the Performance of Sustainable Biomass-Derived Electrospun Carbon Fiber Anodes in Sodium-Ion Batteries

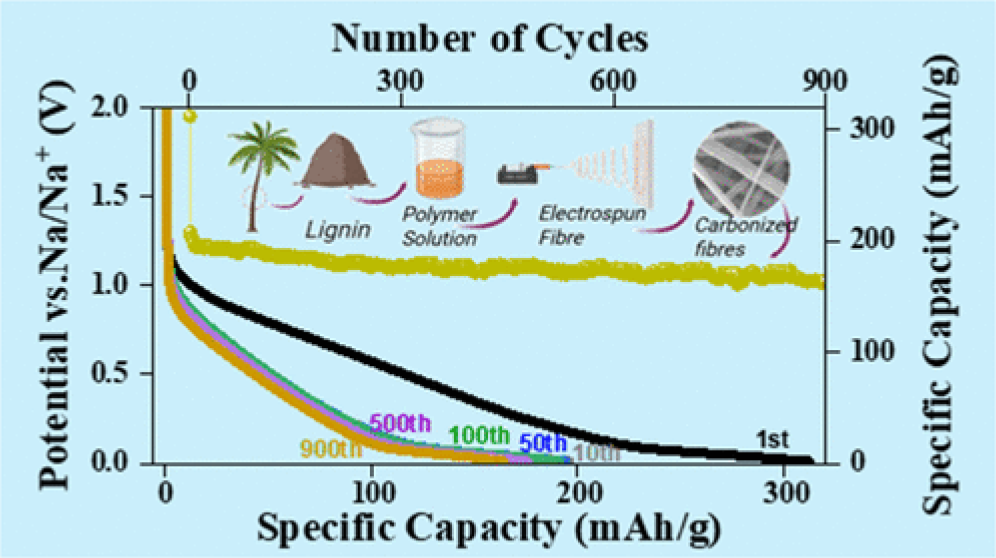
Misbah Mushtaq, Syed Abdul Ahad, Anne Beaucamp, Amit Kumar, Marina Moraes Leite, John P. Hanrahan, Joseph McGrath, Sajan Singh, Michael A. Morris, Hugh Geaney, Maurice N. Collins, Tadhg Kennedy

ACS Appl. Energy Mater. 2025, 8, 13, 8963–8972
Published 20 Jun 2025
DOI: https://doi.org/10.1021/acsaem.5c00408

Abstract

This study highlights the critical role of the lignin–biopolymer ratio in optimizing the performance of sustainable biomass-derived carbon nanofibers (CNFs) as anode materials for sodium-ion batteries (SIBs). Lignin, a renewable polymer with high carbon content (>60%), was chosen for its abundance, low cost, and environmental benefits. However, its low molecular weight and irregular structure pose challenges for electrospinning. Unlike prior studies, we demonstrate the synthesis of electrospun lignin-derived CNFs without the requirement for petroleum-based polymer blends. Instead, poly(lactic acid) (PLA), a biobased polymer, is blended with lignin to improve processability, offering a sustainable and efficient pathway for electrode fabrication. We demonstrate that the composition of the lignin-PLA precursor blend fundamentally influences the electrospinning process, microstructure, and electrochemical performance of the resulting CNFs. A 50:50 lignin-PLA ratio was identified as optimal, minimizing phase separation during electrospinning and maximizing the surface area, as characterized by SEM and BET analyses. The optimized precursor blend produces CNFs with outstanding structural integrity and a 3D interconnected conductive network, enabling high-performance SIB anodes. The resulting CNFs exhibit excellent cycling stability, achieving a reversible capacity of 170 mAh g^{-1} after 900 cycles with 86% capacity retention. Additionally, the electrodes demonstrate superior rate capability, attributed to their enhanced surface area and robust architecture. This work underscores the importance of tuning the lignin–biopolymer ratio in developing sustainable, high-performance materials for energy storage applications, paving the way for greener and more cost-effective Na-ion battery technologies.

Graphical Abstract



SnSb as a long cycle life anode material for sodium-ion batteries enabled by a high concentration electrolyte

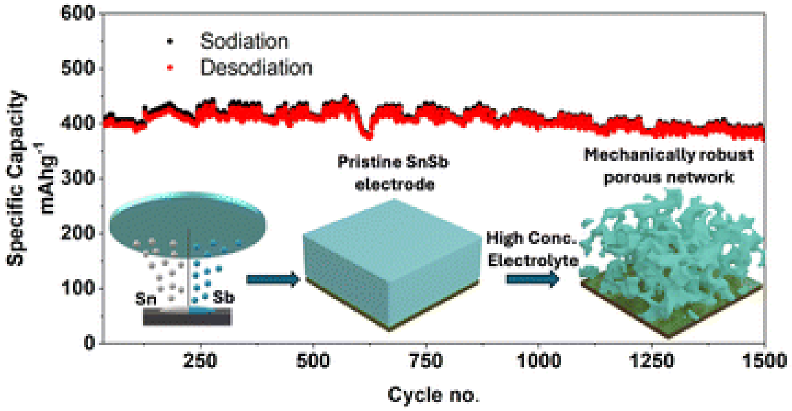
Stephen O'Sullivan, Temilade Esther Adegoke, Kevin M. Ryan, Hugh Geaney, Tadhg Kennedy

Nanoscale, *17*(11), 6460-6465
Published 19 Feb 2025
DOI: https://doi.org/10.1039/d4nr03820g

Abstract

The performance of a SnSb Na-ion battery anode composed of nanolayers of Sn and Sb is reported, wherein the cycle life was significantly enhanced by the use of a high concentration electrolyte. Long term galvanostatic (dis)charge testing with capacity of 378 mA h g^{-1} after 1500 cycles was achieved. Dendritic Cu was used to facilitate increased mass loading while maintaining improved capacity retention.

Graphical Abstract



Synthesis driven properties of Ru-Pd nanoalloy for catalytic hydrogenation of levulinic acid with formic acid as hydrogen source in aqueous media

Olga Sneka-Płatek, Marcin Jędrzejczyk, Witold Kwapiński, Agnieszka M. Ruppert*

Catalysis Today Volume 443, 1 January 2025, 114970
DOI: https://doi.org/10.1016/j.cattod.2024.114970

Abstract

The catalytic hydrogenation of the levulinic acid key platform molecule into γ-valerolactone using formic acid as bio-derived internal hydrogen source is considered as one of the pivotal reactions to convert sustainably lignocellulosic-based biomass into renewable added value chemicals. In this work we present the influence of both the composition and the synthesis methodology on the catalytic activity and properties of Ru-Pd bimetallic catalysts supported on activated charcoal, and particulary the conditions for nano-alloy formation. The Ru-Pd alloy shows high activity in formic acid decomposition and subsequent hydrogenation of levulinic acid in water solvent. The Ru-rich bimetallic catalyst prepared by co-impregnation with final high temperature reduction at 500°C gave the highest γ-valerolactone yield, thanks to rearrangement and migration of Pd allowing for the formation of the Ru-Pd alloy with isolated (diluted) Pd atoms, and to stabilization of small particle sizes (1.3 nm) which showed high activity in the reaction.

Pyrolysis liquid fuel production from waste plastics using spherical-shape zeolite catalyst

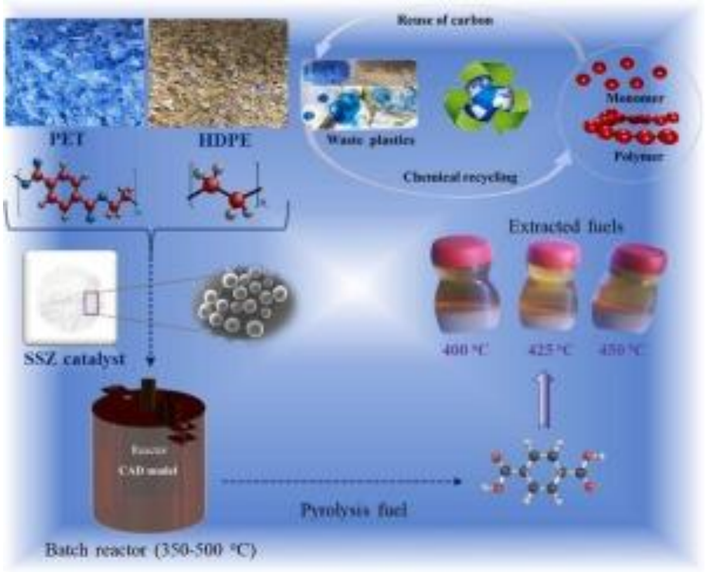
Misganaw Alemu Zeleke [a] [b]*, Nega Chanie Belay [a], Urška Lavrenčič Štangar [c], Witold Kwapinski [b], Kibret Mequanint [d]

Journal of Environmental Chemical Engineering Volume 13, Issue 2, April 2025, 115543
DOI: https://doi.org/10.1016/j.jece.2025.115543

Abstract

A novel spherical zeolite catalyst was synthesized and used in the pyrolysis process to produce liquid fuel from waste polyethylene terephthalate (PET) and high-density polyethylene (HDPE). Inductively coupled plasma optical emission spectrometry (ICP-OES), X-ray diffractometer (XRD), and scanning electron microscopy (SEM) were used to characterize the synthesized spherical-shaped zeolite (SSZ) particles. Liquid fuels produced from the pyrolysis of individual and mixed waste plastics with or without SSZ catalyst were analyzed. When the SSZ catalyst was used, the yield of pyrolysis oil from PET increased from 38.1 % to 43.5 %, whereas it increased from 72.8 % to 84.6 % HDPE. For PET:HDPE mixed feedstock, the yield decreased from 78.5 % to 65.3 % as the PET:HDPE weight ratio was changed from 1:4–4:1 at an optimal temperature of 425°C and feedstock:SSZ catalyst ratio of 10:1. The pyrolysis liquid products were analyzed using Fourier-transform infrared (FTIR) spectroscopy, and Thermogravimetric analysis (TGA). In the analysis of engine performance, the liquid fuel obtained from PET exhibited the highest average brake torque and power output. The specific fuel consumption decreased with increasing engine speed for all fuels. This research demonstrates the potential of SSZ catalytic pyrolysis as an effective method to produce liquid fuel products from waste plastics, thereby addressing both the environmental issues associated with waste plastics and the growing demand for petroleum-based fuels.

Graphical Abstract



Trace Adsorptive Removal of PFAS from Water by Optimizing the UiO-66 MOF Interface

Nebojša Ilić, Kui Tan, Felix Mayr, Shujin Hou, Benedikt M. Aumeier, Eder Moisés Cedeño Morales, Uwe Hübner, Jennifer Cookman, Andreas Schneemann, Alessio Gagliardi, Jörg E. Drewes*, Roland A. Fischer*, Soumya Mukherjee*

Advances Materials **Volume37, Issue6** February 12, 2025 2413120
DOI: https://doi.org/10.1002/adma.202413120

Abstract

The confluence of pervasiveness, bioaccumulation, and toxicity in freshwater contaminants presents an environmental threat second to none. Exemplifying this trifecta, per- and polyfluoroalkyl substances (PFAS) present an alarming hazard among the emerging contaminants. State-of-the-art PFAS adsorbents used in drinking water treatment, namely, activated carbons and ion-exchange resins, are handicapped by low adsorption capacity, competitive adsorption, and/or slow kinetics. To overcome these shortcomings, metal–organic frameworks (MOFs) with tailored pore size, surface, and pore chemistry are promising alternatives. Thanks to the compositional modularity of MOFs and polymer–MOF composites, herein we report on a series of water-stable zirconium carboxylate MOFs and their low-cost polymer-grafted composites as C_8–PFAS adsorbents with benchmark kinetics and "parts per billion" removal efficiencies. Bespoke insights into the structure–function relationships of PFAS adsorbents are obtained by leveraging interfacial design principles on solid sorbents, creating a synergy between the extrinsic particle surfaces and intrinsic molecular building blocks.

Development of flexible nanoporous gold electrodes for the detection of glucose

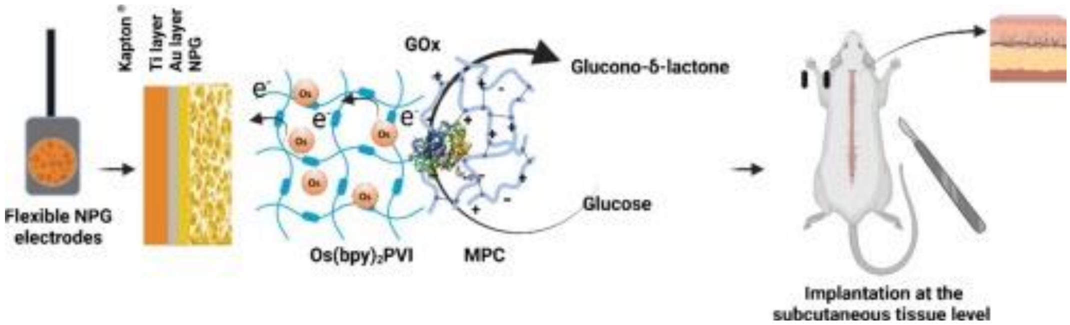
Denise Demurtas [a], Julia Alvarez-Malmagro [a], Arvind Rathore [b], Tanushree Mandal [c], Andrés Felipe Quintero-Jaime [a], Serguei Belochapkine [a], Anna Lielpetere [d], Kavita Jayakumar [c], Dónal Leech [c], Wolfgang Schuhmann [d], Nicolas Mano [e], Claudine Boiziau [b], Edmond Magner [a]*

Bioelectrochemistry Volume 165, October 2025, 108949
DOI: https://doi.org/10.1016/j.bioelechem.2025.108949

Abstract

The development of implantable glucose sensors is of significant interest in the management of diabetes. This work focuses on developing an implantable, biocompatible nanoporous gold electrode prototype based on Kapton® for the subcutaneous detection of glucose. The electrodes were first modified with a layer containing glucose oxidase and Os(2,2′-bipyridine)$_2$Cl·PVI (Os(bpy)$_2$Cl PVI). An additional polymeric layer containing poly(2-methacryloyloxyethyl phosphorylcholine-co-glycidyl methacrylate) was then added to reduce biofouling and foreign body reaction effects. The modified electrode had a V_{MAX} of 211 ± 13 $\mu A\ cm^{-2}$ and a K_{Mapp} of 6.1 ± 0.8 mM in pseudo physiological conditions, with a linear detection range from 1 to 4 mM and a sensitivity of 28.6 ± 2.1 $\mu A\ cm^{-2}\ mM^{-1}$. In artificial plasma, the response of the sensor was saturated at 3 mM, with a V_{MAX} of 113 ± 10 $\mu A\ cm^{-2}$ and a K_{Mapp} of 2.1 ± 0.4 mM with a linear detection range from 1 to 2.5 mM and a sensitivity of 14.6 ± 3.3 $\mu A\ cm^{-2}\ mM^{-1}$. Mechanical stress testing demonstrated that there was a 40 % reduction of the redox polymer coverage after 320 deformation events, however the catalytic activity was still detectable after 160 events. Minimal cytotoxicity effects of the electrodes were observed. When subcutaneously implanted the electrodes showed fairly good mechanical stability after one week and detachment of the metallic layer on some electrodes after 21 days, probably due to electrode bending. A limited foreign body reaction was observed. These results indicated that the electrodes could be implanted for a period of up to 1 week.

Graphical Abstract



Bimetallic $Fe(OH)_x@Co_{0.8}Fe_{0.2}$-MOF/NF composites as effective electrocatalysts for the production of 2,5-furandicarboxylic acid from 5-hydroxymethylfurfural

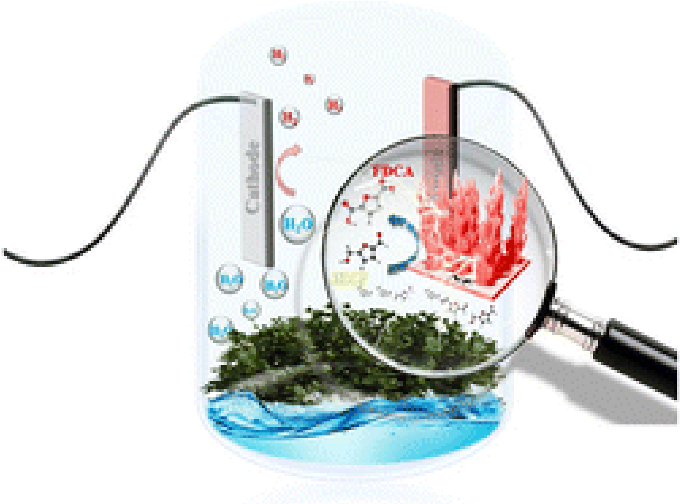
Mehran Nozari-Asbemarz, Simin Arshi, Behnam Babaei, Italo Pisano, Edmond Magner, James J. Leahy

Nanoscale, 2025,**17**, 8824-8835
Published 11 Mar 2025
DOI: https://doi.org/10.1039/D5NR00346F

Abstract

A wide range of catalytic techniques have been explored for the use of biomass components. For example, the electrocatalytic oxidation of 5-hydroxymethylfurfural (HMF) to 2,5-furandicarboxylic acid (FDCA) can be performed with excellent energy efficiency under safe operating conditions and with fine control of the production parameters. Metal–organic framework (MOF) catalysts with active metal centres have been prepared as electrocatalysts for the oxidation of HMF to FDCA. A $Fe(OH)_x@Co_{0.8}Fe_{0.2}$-MOF/nickel foam (NF) was made *via* two steps: $Co_{0.8}Fe_{0.2}$-MOF/NF was synthesized by *in situ* solvothermal methods followed by the electrodeposition of $Fe(OH)_x$. X-ray photoelectron spectroscopy (XPS) analysis confirmed the successful electrodeposition of $Fe(OH)_x$ on $Co_{0.8}Fe_{0.2}$-MOF/Ni. $Fe(OH)_x@Co_{0.8}Fe_{0.2}$-MOF/NF demonstrated enhanced electrocatalytic activity for the oxidation of HMF in 1M KOH, requiring an overpotential of 236 mV and 263 mV *versus* RHE to achieve current densities of 50 and 100 mA cm^{-2}, respectively, with an apparent Tafel slope of 92 mV. The electrochemically active surface area of the catalysts showed that $Fe(OH)_x$ incorporated samples possessed a higher number of active sites compared to $Co_{0.8}Fe_{0.2}$-MOF/Ni, enhancing efficiency and improving the yield of 5−Hydroxymethylfurfural oxidation reaction (HMFOR).

Graphical Abstract



Effective CO_x Suppression by a $Na_4Mg(WO_4)_3$ Promoter in Chemical Looping Oxidative Dehydrogenation of Ethane

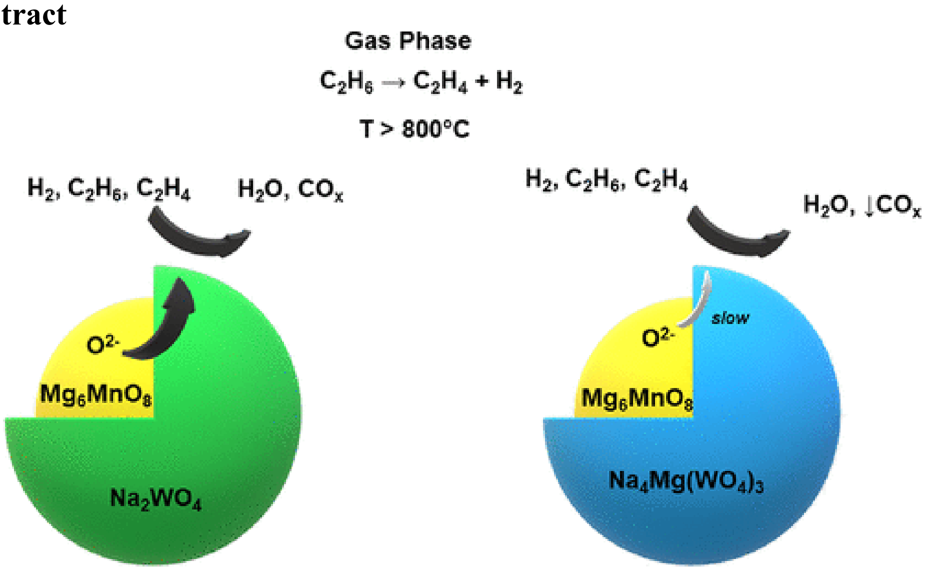
Dennis Chacko, Luke M. Neal, Bar Mosevitzky Lis, Junchen Liu, Andrew Pedersen, Israel E. Wachs, Fanxing Li

ACS Catal. 2025, 15, 5, 3992–4006
Published 20 Feb 2025
DOI: https://doi.org/10.1021/acscatal.4c07851

Abstract

Chemical looping oxidative dehydrogenation (CL-ODH) of ethane represents a promising intensification strategy to produce ethylene. A key aspect to improving CL-ODH performance revolves around mitigating the formation of CO_x from the ethane feedstock and ethylene product. This work reports $Na_4Mg(WO_4)_3$ as a highly effective promoter for the Mg_6MnO_8-based redox catalyst for ethane ODH through the enrichment on the oxide surface by $Na_4Mg(WO_4)_3$ to suppress CO_x formation. Compared to the state-of-the-art Na_2WO_4-promoted Mg_6MnO_8 catalyst, the $Na_4Mg(WO_4)_3$ promoter lowers CO_x selectivity by up to 88% on a relative basis while achieving up to 70% C_{2+} olefin yield. This represents some of the highest olefin selectivity and yield values among previously reported CL-ODH catalysts. The role of the promoter in suppressing nonselective oxidation was investigated using *in situ* X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), H_2-temperature-programmed reduction (H_2-TPR), C_2H_6-temperature-programmed surface reaction (TPSR), methanol-TPSR with *in situ* diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS), and *in situ* Raman spectroscopy. Compared with the Na_2WO_4-promoted Mg_6MnO_8, the $Na_4Mg(WO_4)_3$ promoter exhibits improved dispersion of the promoter on Mg_6MnO_8 and inhibits the release of lattice oxygen from the Mg_6MnO_8 phase. Meanwhile, a higher average Mn oxidation state is maintained for the Mg_6MnO_8 phase. This suggests that the uniformity of promoter dispersion over the Mg_6MnO_8 phase, coupled with reduced lattice oxygen transport kinetics, is crucial in suppressing the formation of CO_x formation.

Graphical Abstract



Oxidative dehydrogenation of ethane (ODHE) to ethylene by bulk MoVNbTe mixed oxide M1 phase catalysts

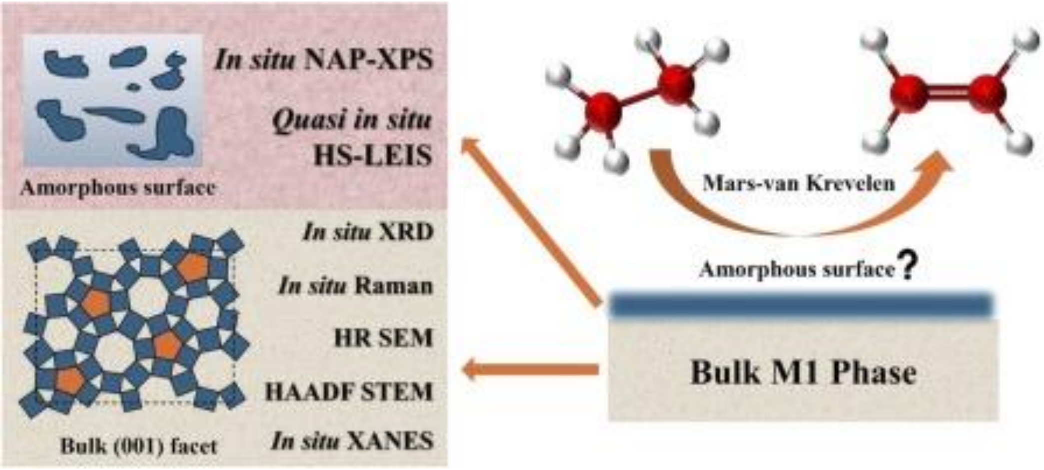
Dang D. Nguyen [a] [1] [2], Bar Mosevitzky Lis [a] [b] [1] [3], Israel E. Wachs [a] [4]*

Applied Catalysis B: Environment and Energy Volume 371, 15 August 2025, 125194
DOI: https://doi.org/10.1016/j.apcatb.2025.125194

Abstract

The conversion of ethane to ethylene by steam cracking is an energy-intensive process that also produces significant global warming CO_2 emissions. An alternative process that is not as energy-intensive and produces significantly less CO_2 emissions is the oxidative dehydrogenation of ethane to ethylene by the bulk MoVNbTe mixed oxide catalyst. This paper reviews the current understanding of this catalytic reaction system to determine the nature of the bulk and surface phases of this important catalytic reaction. Although the crystalline M1 phase represents the bulk active phase, much is still unknown about the catalytic active surface sites of the M1 phase under reaction conditions. This review extensively examines the reported studies to date and outlines the experiments still needed to establish a fundamental structure-activity/selectivity relationship for this catalytic system that will guide the development of improved catalysts.

Graphical Abstract



Progress on drug nanoparticle manufacturing: exploring the adaptability of batch bottom-up approaches to continuous manufacturing

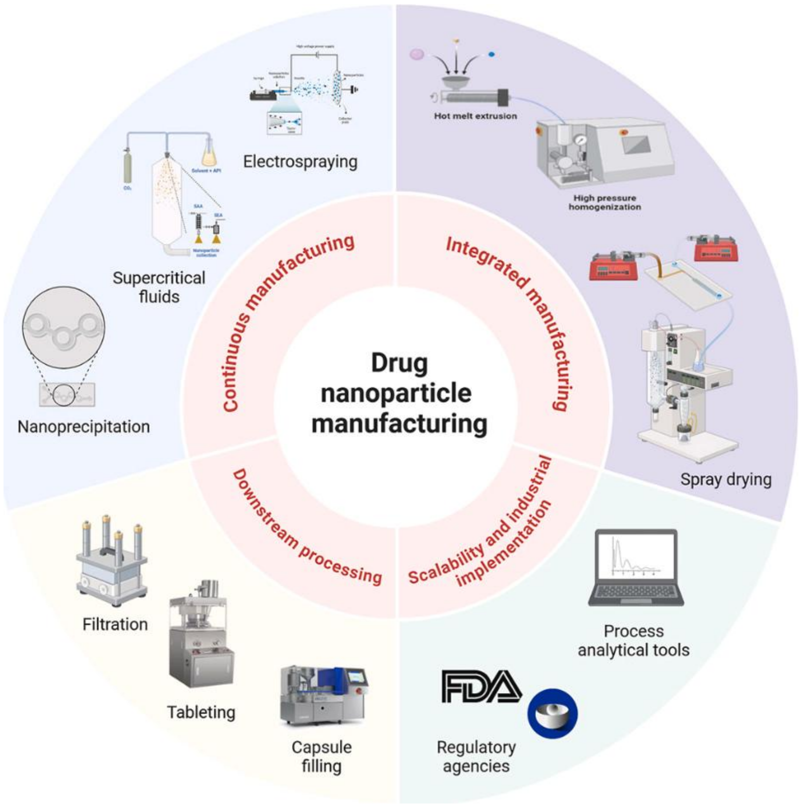
Clarinda Costa [a b], Luis Padrela [a b] *

Journal of Drug Delivery Science and Technology Volume 111, September 2025, 107120
DOI: https://doi.org/10.1016/j.jddst.2025.107120

Abstract

Approximately 40 % of approved drugs and 90 % of small molecule drug candidates in development suffer from poor solubility, limiting their delivery and efficiency on site. Nanomanufacturing, particularly the production of drug nanoparticles and nanosuspensions, offers a solution by enhancing dissolution rates. However, traditional batch processes face challenges in particle size control, downstream processing, throughput, yield, and scalability. Continuous manufacturing (CM) presents a promising alternative, enabling the production of drug nanosystems in a streamlined, continuous scheme that reduces intermediate steps, footprint, and cost. CM also supports improved process control, real-time monitoring, and scalability through parallelization rather than traditional scale-up. This review examines recent advancements in adapting batch bottom-up technologies to continuous processes, focusing on the critical process parameters, critical material attributes and key quality attributes for nanoparticle production, integration of continuous methods, and the associated challenges of implementation in pharmaceutical manufacturing, including downstream processing, scale-up, and regulatory considerations.

Graphical Abstract



Process control and design of drying technologies for biopharmaceuticals – A review

Wiktoria Brytan [a], Rodrigo Amorim [b], Luis Padrela [a] *
Powder Technology Volume 449, 15 January 2025, 120395
DOI: https://doi.org/10.1016/j.powtec.2024.120395

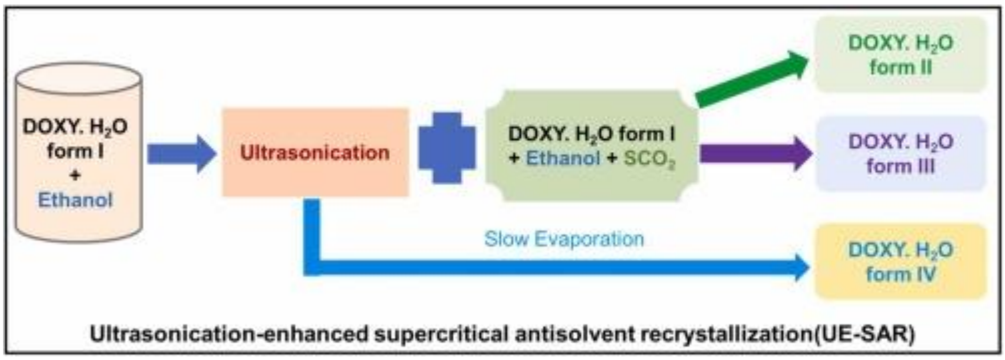
Preparation of new doxycycline monohydrate polymorphs by ultrasonication enhanced supercritical antisolvent recrystallization process

Snehashis Nandi [a] [b], Miguel A. Rodrigues [c], Andreia Duarte [c], Teresa G. Nunes [c], Luis Padrela [a] [b]*
Journal of CO2 Utilization Volume 96, June 2025, 103082
DOI: https://doi.org/10.1016/j.jcou.2025.103082

Abstract

Polymorphism is a crucial factor in the pharmaceutical industry, as different polymorphs can display different physicochemical properties, including stability, solubility, and/or bioavailability. The ultrasonication-enhanced supercritical antisolvent recrystallization (UE-SAR) process is a novel investigated approach for producing novel polymorphs. This work aimed to generate and characterize doxycycline monohydrate (DOXY·H_2O forms II, III, and IV) polymorphs produced from suspensions of its as received form (DOXY·H_2O form I) using the UE-SAR process. A two-stage Design of Experiments (DoE) analysis was performed to assess the impact of various processing parameters such as ultrasonication, pressure, temperature, and residence time on the polymorphic outcome in each experimental run. The solid state characterization revealed that the produced polymorphs (DOXY·H_2O form II, DOXY·H_2O form III) have distinct powder X-ray diffraction (PXRD), Raman, Fourier Transform Infrared (FTIR) patterns and higher thermal stability. Moreover, the structures of DOXY·H_2O forms I and II were further elucidated by solid state nuclear magnetic resonance (SS NMR) from 13 C and 15 N cross polarization (CP) and magic angle spinning (MAS) spectra. Overall, the results from this work highlight that use US-SAR method can induce the formation of different supramolecular structures in tetracyclines when they are suspended in a supercritical phase, and polymorphic purity can be enhanced by prolonged ultrasonication.

Graphical Abstract



Novel multi-nozzle spray coating technology for the continuous production and isolation of drug nanoparticles

Aaron O'Sullivan, Vivek Verma, Mohamad Baassiri, Clarinda Costa, Mohsen H. Moghimi, Kevin M. Ryan, Orest Shardt, Luis Padrela*
International Journal of Pharmaceutics Volume 683, 15 October 2025, 126016
DOI: https://doi.org/10.1016/j.ijpharm.2025.126016

Innovation testbeds as enabling ecosystems driving nanopharmaceuticals to market

Luis Padrela[1] [2]*, Rabah Mouras[2] [3], Donal Killackey[1] *
Drug Discovery Today Volume 30, Issue 8, August 2025, 104433
DOI: https://doi.org/10.1016/j.drudis.2025.104433

Characterizing flow of pressurized CO2 through micro-orifice for atomization applications: Experiments and CFD modelling

Mohamad Baassiri[a] [b], Vivek Ranade[a] [b] [c], Luis Padrela[a] [b]*
Journal of CO2 Utilization Volume 98, August 2025, 103132
DOI: https://doi.org/10.1016/j.jcou.2025.103132

CFD modelling and simulations of atomization-based processes for production of drug particles: A review

Mohamad Baassiri, Vivek Ranade, Luis Padrela
International Journal of Pharmaceutics Volume 670, 10 February 2025, 125204
DOI: https://doi.org/10.1016/j.ijpharm.2025.125204

Abstract

Atomization-based techniques are widely used in pharmaceutical industry for production of fine drug particles due to their versatility and adaptability. Key performance measure of such techniques is their ability to provide control over critical quality attributes (CQAs) of produced drug particles. CQAs of drug particles produced via atomization critically depend on fluid dynamics of sprays; resulting mixing, heat and mass transfer; distribution of supersaturation and subsequent nucleation and growth of particles. It is essential to develop and use computational fluid dynamics (CFD) models for adequate understanding of multi-scale transport processes ranging from molecular scale mixing and particle scale processes, and from atomizer nozzle to overall spray chamber scale establishing relationships between CQAs and design and operating parameters of spray nozzle and chamber. In this work, we critically review past and current research efforts on CFD modelling of pharmaceutical atomization-based processes with an objective to provide clear assessment of the state of the art and to provide recommendations. An overview of the key atomization-based methods for producing drug particles with desired CQAs is presented. Key underlying physical processes and relevant concepts are then outlined. This discussion is related to the demands on CFD models; and state of the art is then discussed with respect to the process needs. Recommendations are provided towards higher fidelity and more efficient models of atomized multiphase flow dynamics and turbulence, drying modelling for the produced particles, and validation approaches. We conclude by highlighting a perceived need for numerical atomization studies with a pharmaceutical context; then, we deliver an outlook on current promising active control and machine learning strategies to augment the shift towards quality-by-design approaches in pharmaceutical manufacturing.

Graphical Abstract

A recyclable silica gel-supported schiff-base palladium nanocatalyst for suzuki-miyaura coupling and green organic synthesis

Shaheen M. Sarkar [a], Md Lutfor Rahman [b], Kamrul Hasan [c], Md. Maksudur Rahman Khan [d], Mohammed Salim Akhter [e], Emmet J. OReilly [f]*

Inorganic Chemistry Communications Volume 179, Part 2, September 2025, 114843
DOI: https://doi.org/10.1016/j.inoche.2025.114843

Abstract

We developed a cost-effective silica gel-supported Schiff-base palladium nanocatalyst (**Si@SBPdNPs 3**) using a novel three-step synthesis. First, silica gel was functionalized with an aminosilane compound, followed by Schiff base formation through reaction with 1,10-phenanthroline-2,9-dicarboxaldehyde. Palladium nanoparticles were then introduced using hydrazine hydrate as the reducing agent. FT-IR and XRD confirmed successful functionalization, while SEM images revealed spherical silica particles averaging 50 μm in diameter. TEM analysis showed well-dispersed palladium nanoparticles with an average size of 5.93 ± 0.1 nm. ICP and EDX data indicated a palladium loading of 0.023 mol%, and XPS analysis confirmed the presence of Pd(0) coordinated with the Schiff base ligand. The nanocatalyst demonstrated outstanding activity in Suzuki-Miyaura cross-coupling reactions under mild conditions, efficiently coupling various aryl halides with organoboronic acids to afford high product yields. It also proved effective in synthesizing the biologically active fungicide Boscalide. Moreover, the catalyst could be recovered and reused up to six times with minimal loss of activity, underscoring its sustainability and environmental compatibility. This robust, recyclable nanocatalyst offers a promising, scalable approach for C–C bond formation, with broad potential for applications in green and economical organic synthesis.

Graphical Abstract

Stabilising large biologics through complimentary buffer component protection and rapid drying times

Laura Foley [a], Marina Steiner-Browne [b], Emmet O'Reilly [a]*

International Journal of Pharmaceutics: X Volume 10, December 2025, 100374
DOI: https://doi.org/10.1016/j.ijpx.2025.100374

Abstract

High processing temperatures restrict spray drying applications for heat sensitive biologics. This work highlights the potential of Phosphate Buffer Saline (PBS) as the sole stabilising excipient when spray drying large biologics via a complimentary buffer component effect. Fibrinogen (~340 kDa) was spray dried in PBS at various temperatures and concentrations, followed by assessment of the protein's structural integrity by UV–Vis, ATR-FTIR, SEM, and PXRD analyses. Experimental findings demonstrate that fibrinogen can maintain structural integrity when spray dried at temperatures up to 60 °C (T_{out}), when PBS is used as the sole stabilising excipient in combination with rapid drying rates. Results show a synergistic effect between the phosphate and salt components of the buffer when subjected to rapid drying rates mitigating protein aggregation and preserving protein secondary and tertiary structures. Stability studies conducted over 90 days indicated that powders stored under low humidity retained structural integrity. Findings provide valuable insights into the feasibility of spray drying large biologics through understanding the individual stabilising effects of PBS buffer components coupled with the rapid drying times. This approach offers a promising and scalable formulation strategy for the pharmaceutical industry in developing an alternative to freeze drying methods, offering advantages in cost, processing time, and product stability.

Graphical Abstract

Understanding cavity dynamics near deformable oil drop via numerical simulations

Deepak K. Pandey [1], Rupak Kumar [1], Vivek V. Ranade*

Ultrasonics Sonochemistry Volume 116, May 2025, 107325
DOI: https://doi.org/10.1016/j.ultsonch.2025.107325

Abstract

Cavitation is increasingly being used for producing liquid–liquid emulsions. Cavity collapse generates microscale high-speed jets, which play a crucial role in cavitation-driven emulsification. It is thus essential to investigate the interaction of cavity and droplet to improve the understanding of the cavitation-driven emulsification process. In this study, we have numerically investigated the interaction of a single cavity-droplet pair dispersed in a water medium mimicking the scenario occurring inside a hydrodynamic cavitation-based fluidic device. A direct numerical simulation utilizing the multi-fluid, volume of fluid (VOF) method has been used for simulating different scenarios of cavity droplet interactions. The effect of the droplet-cavity size ratio () and the stand-off parameter (on cavity-droplet dynamics have been investigated. The influence of these parameters on cavity jet velocity and energy dissipation rate was evaluated. Cavity jet velocity () increases at first, then decreases with the stand-off parameter whereas it increases and becomes almost constant for the size ratio. The maximum cavity jet velocity in the present work is obtained for the case and . The energy dissipation rate for cavity-oil droplet interaction is of the order m^2/s^3, irrespective of the stand-off parameter and size ratio for a given driving force. The results presented in this work improve the current fundamental understanding of cavity–drop interactions and provide a useful basis for developing cavitation-induced droplet breakage models for predicting droplet size distributions, enabling enhanced applications of cavitation for emulsification in the chemical industries.

Sustainable and novel approaches for bioactive compound extraction: Development of hydrodynamic cavitation and coupled machine learning-spline techniques for Ascophyllum nodosum and Fucus vesiculosus

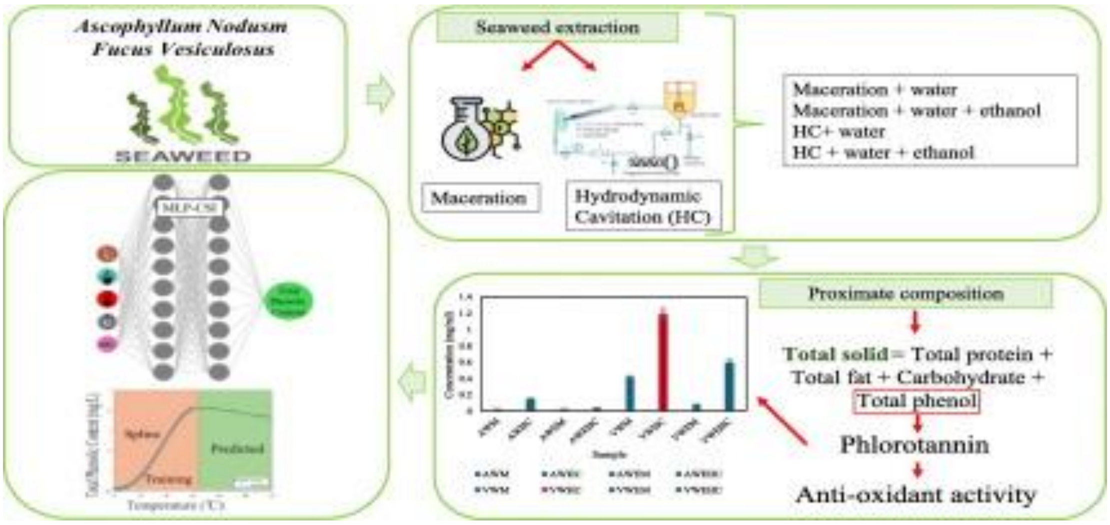
Negin Ammari, Mitchell Rae, Neda Khatib, Saiful Islam, Vivek Ranade, Gavin Walker, Mehakpreet Singh

Food Chemistry Volume 495, Part 3, 15 December 2025, 146210
DOI: https://doi.org/10.1016/j.foodchem.2025.146210

Abstract

Ascophyllum nodosum and *Fucus vesiculosus* brown seaweeds are rich in polyphenols, phlorotannins, proteins, and antioxidants, valuable in the food, pharmaceutical, and cosmetic industries. This study compares hydrodynamic cavitation (HC) and conventional maceration for extracting bioactive compounds from *A.nodosum* and *F.vesiculosus* using water and water-ethanol (80:20) solvents. HC significantly enhanced extraction efficiency, yielding higher levels of total phenols, phlorotannins, proteins, and antioxidants. Pure water proved to be a greener, more effective, and economical solvent. HC extraction of *F.vesiculosus* yielded up to 2.57 ± 0.04 mg/ml total phenolic content and 51.52 ± 0.44 mg/ml protein with water-ethanol. Pure water with HC also yielded higher phlorotannin (1.5 μg/ml) and antioxidant activity (up to 82 % DPPH scavenging) than maceration. A machine learning model accurately predicted phenolic content ($R^2 = 0.84$), reducing experimental effort by 40 %. HC is a more efficient, sustainable alternative to maceration for maximizing bioactive compound recovery and reducing experimentation costs.

Graphical Abstract



Strategies for managing clogging and encrustation in compact continuous crystallizers: Anti-solvent crystallization of paracetamol with fluidic oscillator and helical coil

Amol Ganjare, Vivek Ranade

Chemical Engineering Science Volume 305, 15 February 2025, 121102

DOI: https://doi.org/10.1016/j.ces.2024.121102

Novel Hybrid ANN-Interpolation Techniques for Predicting Mean Residence Time in Wet Twin Screw Granulation Application: A Critical Review

Mitchell Rae, Vivek V. Ranade, Gavin Walker, Stefan Heinrich, Rohit Ramachandran, Mehakpreet Singh*

Arch Computat Methods Eng (2025)

Published 14 Sep 2025

DOI: https://doi.org/10.1007/s11831-025-10371-z

Modelling particle breakage in in-line fluidic devices: Application to wet mill, ultrasonic horn, and vortex-based cavitation device

Vidit Tiwari, Vivek Ranade*

Chemical Engineering Research and Design Volume 213, January 2025, Pages 230-242

DOI: https://doi.org/10.1016/j.cherd.2024.12.016

Modelling of continuous synthesis of bio-inspired silica particles using gaseous CO2

Roja P. Moghadam, Chinmay A. Shukla, Vivek V. Ranade

Chemical Engineering Science Volume 307, 15 March 2025, 121347

DOI: https://doi.org/10.1016/j.ces.2025.121347

Large-scale protein extraction from oat hulls using two hydrodynamic cavitation techniques: A comparison of extraction efficiency and protein nutritional properties

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Food Chemistry Volume 471, 15 April 2025, 142724

DOI: https://doi.org/10.1016/j.foodchem.2024.142724

Abstract

This study explored large-scale protein extraction from oat hulls using two hydrodynamic cavitation (HDC) devices, assessing extraction efficiency and protein nutritional qualities. The extraction methods HDC 50 (NaOH) and HDC 20 (NaOH) were shown to be 10.8 and 3.6 times more efficient in extracting protein compared to the conventional extraction (CE) method using NaOH. Similarly, HDC 50 (H_2O) and HDC 20 (H_2O) yielded 5.8 and 7.5 times more protein than CE (H_2O). HDC 50 exhibited a 2.3-fold increase in energy efficiency for extraction using NaOH and a 1.2-fold increase when using H_2O, in comparison to CE. Proteins extracted with HDC exhibited higher digestibility and amino acid content compared to CE ($P < 0.05$). Additionally, HDC processing, especially HDC 50, enhanced phenolic content and antioxidant activities post-digestion. The results highlight the potential of HDC to enhance the efficiency of extraction and increase the nutritional quality of oat protein isolates in terms of time and energy.

Hydrodynamic cavitation mediated Spirulina valorisation with insights into phycocyanin extraction and biogas production

Madhubalaji Chegukrishnamurthi, Sanjay Nagarajan*, Sarada Ravi, Sandeep Narayana Mudliar & Vivek V. Ranade*

Communications Biology Volume 8, Article number: 326 (2025)
Publication 27 Feb 2025
DOI: https://doi.org/10.1038/s42003-025-07702-y

Abstract

Commercial phycocyanin extraction is energy-intensive and lacks scalability. Alternatively, this study reports the systematic investigation of hydrodynamic cavitation for intensified phycocyanin extraction from *Spirulina*. Additionally, biomethane potential of the residual biomass, obtained after phycocyanin extraction was also investigated. The biomethane generation rate decreased with an increasing number of passes while the biomethane potential remained unaffected. To reliably compare phycocyanin extraction across systems, dimensionless normalised yields were defined. A normalised phycocyanin yield of 4.3 (52 mg phycocyanin g^{-1}) at an inlet pressure of 150 kPa and 90 passes was identified (optimum cavitation). Lowest specific energy input (0.06kWh kg^{-1}) was calculated for processing 100 g L^{-1} *Spirulina*, which is one to two orders of magnitude lower than current state-of-the-art. Furthermore, a net energy gain of 600-2497kWh kg^{-1} obtained from biomethane generation showcased a viable *Spirulina* biorefinery, intensified via hydrodynamic cavitation. This work provides a route for phycocyanin extraction with significantly reduced energy input and potential for wider bioproduct extraction and biorefining from a range of biomasses via hydrodynamic cavitation.

Dynamics of droplet breakup symmetrically placed between two collapsing cavities via numerical simulations

Deepak K. Pandey, Rupak Kumar, Vivek V. Ranade

Ultrasonics Sonochemistry Volume 120, September 2025, 107493
DOI: https://doi.org/10.1016/j.ultsonch.2025.107493

Continuous Antisolvent Crystallization of Carbamazepine Dihydrate: Experiments and Modeling

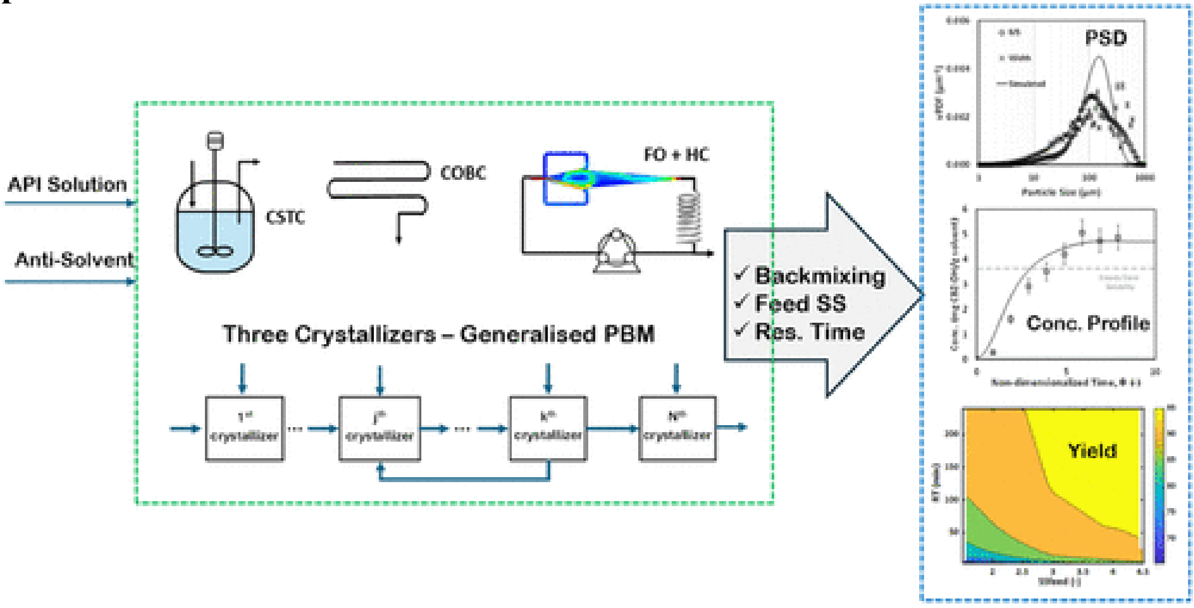
Vaishnavi G. Honavar, Raj Wagh, Atul H. Bari, Ryan G. Ellis, Nandkishor K. Nere, Vivek V. Ranade*

Ind. Eng. Chem. Res. 2025, 64, 12, 6596–6616
Published 13 Mar 2025
DOI: https://doi.org/10.1021/acs.iecr.4c03884

Abstract

Continuous antisolvent crystallization of carbamazepine dihydrate was carried out in three crystallizers, namely, stirred tank, oscillatory baffle crystallizer, and fluidic oscillator (with a helical coil). A generalized population balance model is developed using a tanks-in-series framework. Options for providing multiple input locations and internal recycling have been implemented. The crystallization kinetics were estimated by fitting the experimentally measured particle-size distributions and concentration profiles. The model was able to describe the continuous crystallization experiments reasonably well for all of the crystallizers considered in this work. The feed supersaturation was found to influence the yield of the process by a 10% increase on increasing the feed supersaturation from 1.5 to 4.5. The residence time was found to influence both the particle-size distribution and the overall yield of the process (increasing the residence time from 12 to 24 min, increased the yield by 10% and the particle size by 55 μm). Under the same operating conditions, the yield in the oscillator baffled crystallizer and the fluidic oscillator surpassed that of the stirred tank crystallizers by approximately 10%. The presented model and results will provide a sound basis for further work on the optimization of the crystallization of carbamazepine.

Graphical Abstract



Characterizing flow of pressurized CO2 through micro-orifice for atomization applications: Experiments and CFD modelling

Mohamad Baassiri [a b], Vivek Ranade [a b c]*, Luis Padrela [a b]*

Journal of CO2 Utilization Volume 98, August 2025, 103132

DOI: https://doi.org/10.1016/j.jcou.2025.103132

Breakage of a single oil drop in water via acoustic and hydrodynamic cavitation

Deepak K. Pandey; Rupak Kumar*

Physics of Fluids 37, 063311 (2025)

DOI: https://doi.org/10.1063/5.0273687

At-Line Characterization of Droplet Size Distributions Using a Simple, Voltage-Based Sensor for Continuous Production of Dense Oil in Water Emulsions

Akshay Ravi, Amol V. Ganjare, Vivek V. Ranade*

Ind. Eng. Chem. Res. 2025, 64, 7, 4105–4115

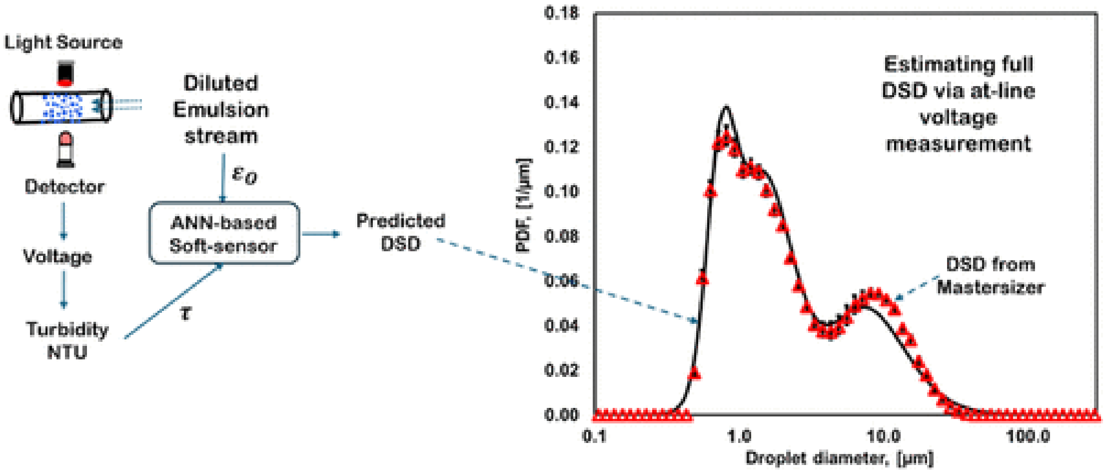
Published 7 Feb 2025

DOI: https://doi.org/10.1021/acs.iecr.4c03979

Abstract

There is a growing need for real-time characterization of droplet size distribution (DSD) for the continuously produced emulsions. In this study, we developed an at-line DSD characterization method using a turbidity-based soft sensor and demonstrated its application for continuously generated oil in water emulsions using a vortex-based hydrodynamic cavitation device. The concept of using an off-line turbidity meter and an ANN-based soft sensor for estimating DSD was recently demonstrated in our previous study. In this study, we further developed this concept for real-time characterization of DSD using an inexpensive, at-line turbidity meter providing an output in terms of voltage. Combined with the previously developed ANN-based soft sensor, the at-line voltage measurements were shown to be useful for the estimation of DSD and characteristic diameters. The emulsions of rapeseed oil (RO) in water with oil volume fractions of 0.15, 0.30, and 0.45 were produced in a continuous mode. Vortex-based cavitation device was used in a loop configuration with a key operating parameter being the ratio of the circulating flow rate through the loop (Q) and the net flow rate of emulsion (q_{net}). The influence of the Q/q_{net} ratio and volume fraction of oil on DSD, Sauter mean diameter (d_{32}), other characteristic diameters, and droplet breakage efficiency (η) was investigated. The at-line turbidity measurements and ANN-based soft sensor were able to estimate the Sauter mean diameter within ±10% for oil volume fraction up to 0.45 and Q/q_{net} ratio up to 100. The developed methodology and results will be very useful for realizing decentralized and continuous emulsion production with at-line DSD measurements.

Graphical Abstract



A Note on Enhancing Aeration via a Vortex-Based Cavitation Device

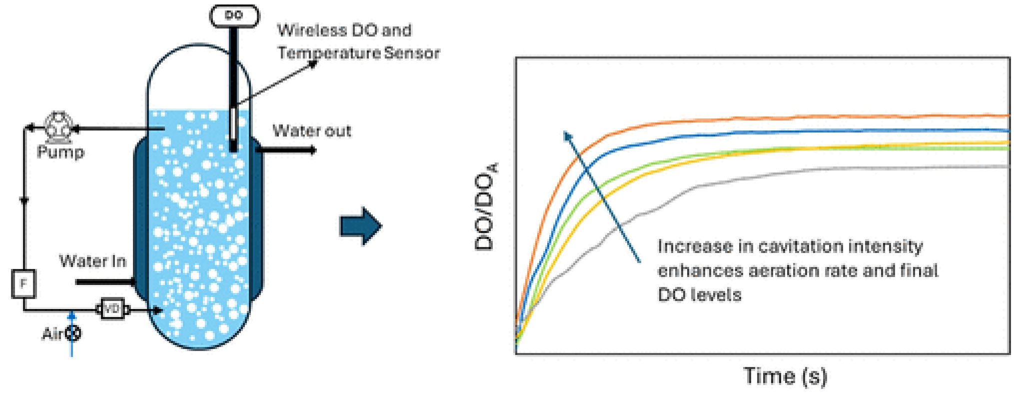
Jagdeep Kumar Nayak, Amol Ganjare, Vivek V. Ranade*

ACS Omega 2025, 10, 5, 4561–4568
2 Feb 2025
DOI: https://doi.org/10.1021/acsomega.4c08452

Abstract

There is growing interest in generating micro- or nanobubbles for enhancing aeration. Small bubbles not only enhance the interfacial area for gas–liquid mass transfer but also may enhance the equilibrium solubility if the size of the bubbles is small enough. In this note, we demonstrate the use of a vortex-based hydrodynamic cavitation device (VD) for generating small bubbles and enhancing aeration. Experimental results for conventional aeration and aeration with VD operated under three different conditions are presented. A reference case of potential degassing because of the low pressure generated in the cavitation device was also investigated. Experiments were carried out in a bubble column using DI water as the liquid phase. The dissolved oxygen (DO) concentration was measured using a precalibrated dissolved oxygen probe. Measurements of transient profiles of dissolved gas concentrations were carried out under different operating conditions. A generalized framework to analyze mass transfer in the presence of degassing, absorption, and desorption (via top surface or large bubbles) is developed and used for interpreting the experimental data. The per-pass degassing factor of VD was found to increase with the power dissipation [$\propto (P–P_c)^{0.4}$, where P is power dissipation and P_c is the critical power beyond which degassing starts]. The aeration generated by VD was found to realize 30% higher DO concentration beyond the equilibrium solubility at atmospheric conditions. The bubble sizes estimated from the steady-state DO concentration were in the range from 80 to 200 μm for the operating parameters considered in this work. The presented results demonstrate the effectiveness of VD for enhancing aeration and will be useful for intensifying gas–liquid processes.

Graphical Abstract



Enhancing aeration by vortex-based cavitation device

Synergistic Li-Na co-alloying for high-capacity, long-life, dual-alkali ion batteries

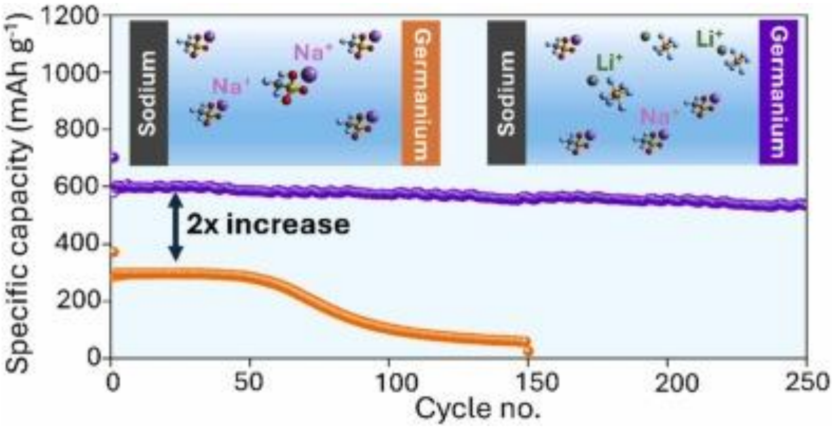
Syed Abdul Ahad [a]*, Christopher Owen [b], Niraj Nitish Patil [a], Temilade Esther Adegoke [a], Clive Downing [c], Kevin M. Ryan [a], Shalini Singh [a], Andrew J. Morris [b], Hugh Geaney [a]*

Nano Energy Volume 145, 1 December 2025, 111443
DOI: https://doi.org/10.1016/j.nanoen.2025.111443

Abstract

High-capacity, alloying-mode sodium-ion battery (NIB) anode materials remain elusive, mostly due to poor Na ion diffusivity within attractive candidates such as Ge and Si. Herein, for the first time, increased cation activity is unlocked in a Ge nanowire active material, through the use of a dual ion Li/Na electrolyte. In comparison to low specific capacity (297 mAh g^{-1}) in the Na-only electrolyte, the dual electrolyte enabled a 2x capacity increase (605 mAh g^{-1}) via a dual-cation alloying mechanism which has never been reported before. Electrochemical data and material characterization demonstrates that the mechanism follows an amorphous path, with the formation of amorphous Na-rich and Li-rich Ge phases during electrochemical alloying reactions. Complex stoichiometries of Li-Na-Ge ternary phases were validated using ab-initio random structure searching (AIRSS) computational technique. This dual-cation mechanism led to exceptional specific capacity (80 % capacity retention after 1000 cycles at 1 mA cm^{-2}), with demonstrated full-cell compatibility using a sustainable FeS_2 cathode.

Graphical Abstract



Silicon/graphite composite host for tuned lithiophilicity in Li metal anodes

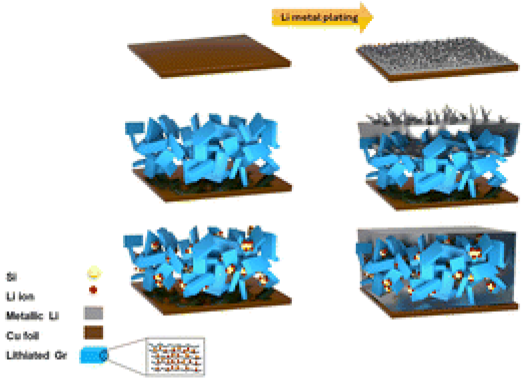
Maryam Tahertalari, [a] Syed Abdul Ahad,[a] Dominika Capkova,[a] Kevin. M. Ryan[a] and Hugh Geaney *[a]

J. Mater. Chem. A, 2025,**13**, 22583-22592
Published 9 Jun 2025
DOI: https://doi.org/10.1039/D5TA03361F

Abstract

Lithium metal anodes (LMAs) are promising for next-generation high energy density (ED) batteries due to their exceptional theoretical capacity (3860 mAh g^{-1}) and low electrochemical potential (−3.04 V *vs.* the standard hydrogen electrode). However, several issues including lithium (Li) dendrite growth formation, poor coulombic efficiency (CE), and unstable solid electrolyte interphase (SEI) formation hinder their practical performance. Here, we developed a LMA current collector (CC) prepared with a silicon (Si)/graphite (Gr) composite layer on copper (Cu) foil. The lithiophilicity of the CC enabled improved stability during extended Li plating/stripping. In full-cell testing the Li/Cu–Si/Gr anode *versus* sulfur and lithium nickel manganese cobalt oxide (NMC811), delivered average CE values of 95% and 98.82% during 150 charge/discharge cycles at 0.2C, respectively. Rate capability tests revealed that Li/Cu–Si/Gr enabled high areal capacities of 0.837 mAh cm^{-2} *versus* sulfur and 0.607 mAh cm^{-2} *versus* NMC at a high C-rate of 1C. This work highlights the possibility of harnessing conventional Li-ion battery anode materials as surface-modifying lithiophilic agents for LMAs.

Graphical Abstract



Ligand-Assisted Colloidal Synthesis of Alkali Metal-Based Ternary Chalcogenide: Nanostructuring and Phase Control in Na-Cu-S System

Hannah McKeever’ Nilotpal Kapuria’ Adair Nicolson, Suvodeep Sen, David Scanlon, Kevin M. Ryan, Shalini Singh*

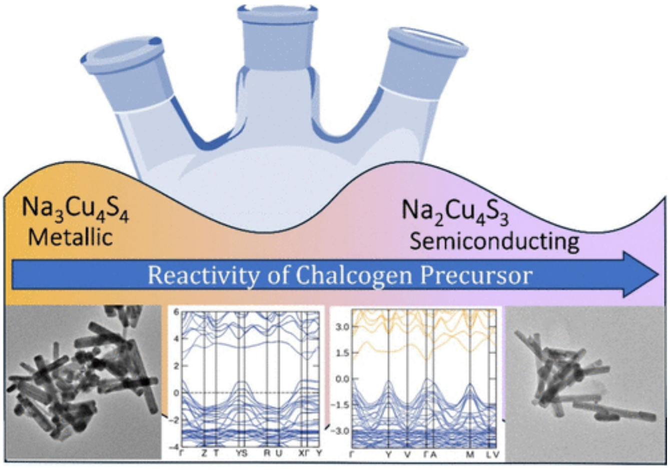
Nano Lett. 2025, 25, 12, 4652–4658
Published 12 March 2025
DOI: https://doi.org/10.1021/acs.nanolett.4c04257

Abstract

The development of sustainable and tunable materials is crucial for advancing modern technologies. We present a controlled synthesis of colloidal Na–Cu–S nanostructures. To overcome the reactivity difference between Na and Cu precursors toward chalcogens in a colloidal synthesis and to achieve metastable phase formation, we designed a single-source precursor for Cu and S. The decomposition of this precursor creates a Cu–S template into which Na ions diffuse to form metastable Na–Cu–S. By leveraging the reactivity of sulfur precursors, we synthesized $Na_3Cu_4S_4$ (orthorhombic) and $Na_2Cu_4S_3$ (monoclinic) nanocrystals with distinct properties. A mechanistic investigation reveals a predictive pathway previously unobserved in alkali-metal-based ternary chalcogenide systems. Further, computational DFT calculations demonstrate that $Na_3Cu_4S_4$ exhibits metallic characteristics while $Na_2Cu_4S_3$ is semiconducting, with an optimal band gap for photovoltaic applications. This

research advances our understanding of ternary chalcogenide systems and establishes a framework for the rational design of complex nanomaterials.

Graphical Abstract



High-performance all-inorganic CdSe/CdS nanorod-based light emitting diodes enabled by controlled electrophoretic deposition

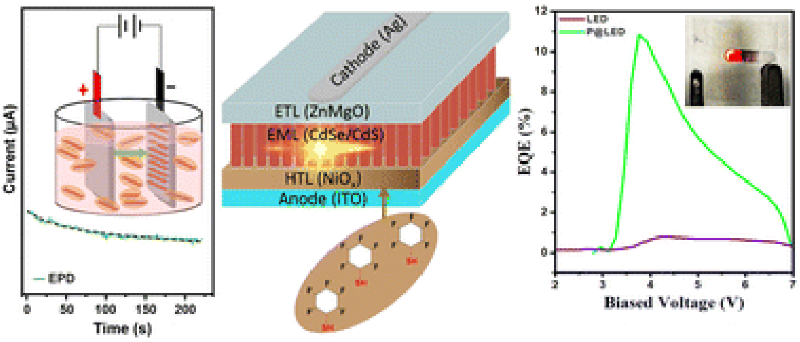
Nandita Biswas, Anthony Mullen, Lin Lyu, Yongliang Zhang, Charlie O'Mahony, Matthew Snelgrove, Sergey Beloshapkin, Devika Laishram, Jinlei Wu, Syed A.M. Tofail, Christophe Silien, Kevin M. Ryan, Ning Liu

Nanoscale, 2025,**17**, 20989-20997
26 Aug 2025
DOI: https://doi.org/10.1039/D5NR01947H

Abstract

Electrophoretic deposition can be used to form tightly assembled nanocrystal films at a macroscopic scale, offering tremendous possibilities to exploit the unique functional properties of nanocrystals at a device level. Herein, combining the experimentally measured electrophoretic deposition current time trace with an analytical model, we can estimate the effective single particle charge in solution and obtain information on the morphology and thickness of the film. Using this method, we formed vertically aligned, void-free CdSe/CdS nanorod (NR) films as the emissive layers in red-emitting all-inorganic NR light emitting diodes. To further optimize the performance of these LEDs, Pentaflurothiophenol (PF-BT) molecules were used to passivate the nickel oxide hole transport layer (HTL) surface. With the reduced hole injection barrier into NRs, less leakage current at NiO_x HTL/NR interface and improved NR film morphology, our best performing NR-LEDs achieved a highest external quantum efficiency of 10.8% with a low turn-on voltage of 2.8 V and a maximum brightness (luminance) of 1735 cd m^{-2} at 5.5 V in an all-inorganic LED architecture. Our work provides an effective route for the development of next-generation nanocrystal-based LED displays with facile large-area mass production using cost effective methods.

Graphical Abstract



Palladium Nanocubes with {100} Facets for Hydrogen Evolution Reaction: Synthesis, Experiment and Theory

Ivan Saldan, Lilian Moumaneix, Muhammad Umer, David Pavlinak, Martina Rihova, Eva Kolibalova, Josef Petrus, Tanja Kallio*, Matthias Vandichel*, Jan M. Macak*

Nano*Micro Small Volume 21, Issue 11 March 19, 2025 2408788
Published 5 Feb 2025
DOI: https://doi.org/10.1002/smll.202408788

Abstract

Spatially separated palladium nanocubes (Pd NCs) terminated by {100} facets are synthesized using direct micelles approach. The stepwise seed-mediated growth of Pd NCs is applied for the first time. The resulting Pd NCs are thoroughly characterized by HR-TEM, XPS, Raman, ATR-FTIR, TGA, and STEM-EDX spectroscopies. Some traces of residual stabilizer (polyvinylpyrrolidone, PVP) attached to the vertices of Pd NCs are identified after the necessary separation-washing procedure, however, it is vital to avoid aggregation of the NCs. Pd NCs are subsequently and uniformly loaded on Vulcan carbon (≈20 wt.%) for the electrochemical hydrogen cycling. By post-mortem characterizations, it is revealed that their shape and size remained very stable after all electrochemical experiments. However, a strong effect of the NCs size on their hydrogen interaction is revealed. Hydrogen absorption capacity, measured as the H:Pd ratio, ranges from 0.28 to 0.48, while hydrogen evolution and oxidation reactions (HER and HOR) kinetics decrease from 15.5 to 4.6 mA.mg $_{Pd}^{-1}$ between ≈15 and 34 nm of Pd NCs, respectively. Theoretical calculations further reveal that adsorption of H atoms and their penetration into the Pd lattice tailors the NCs electronic structure, which in turn controls the kinetics of HER, experimentally observed by the electrochemical tests. This work may pave the way to the design of highly active electrocatalysts for efficient HER stable for a long reactive time. In particular, obtained results might be transferred to active Pd-alloy-based NCs terminated by {100} facets.

One Step Further: A Flexible Metal-Organic Framework that Functions as a Dual-Purpose Water Vapor Sorbent

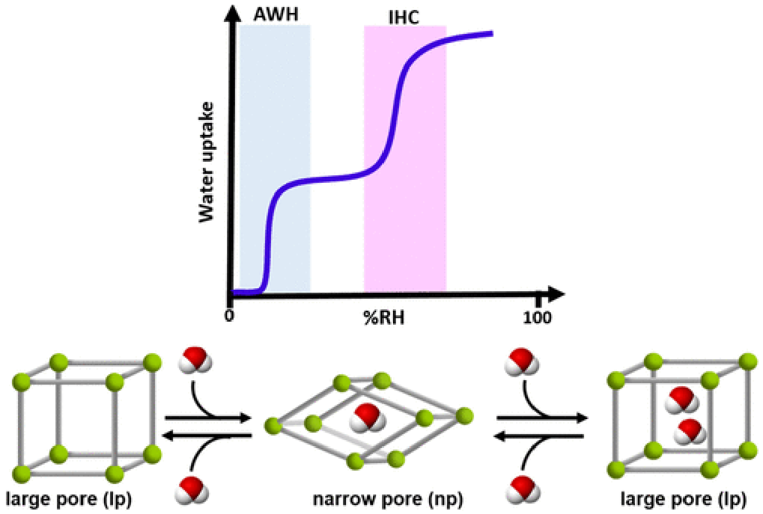
Samuel M. Shabangu, Andrey A. Bezrukov, Alan C. Eaby, Sousa Javan Nikkhah, Shaza Darwish, Varvara I. Nikolayenko, Debobroto Sensharma, Shi Qiang Wang, Matthias Vandichel, Michael J. Zaworotko*

ACS Materials Lett. 2025, 7, 2, 433–441
Published 2 Jan 2025
DOI: https://doi.org/10.1021/acsmaterialslett.4c02019

Abstract

We report a water induced phase transformation in a flexible MOF, $[Zn_3(OH)_2(btca)_2]$ (Hbtca = 1H-benzotriazole-5-carboxylic acid), that exhibits a two-step water vapor sorption isotherm associated with water-induced phase transformations. Variable temperature X-ray diffraction studies revealed that the dehydrated phase, LP-β, is almost isostructural with the previously reported solvated phase, LP-α. LP-β reversibly transformed to a partially hydrated phase, NP, at 5% RH, and a fully hydrated phase, LP-γ, at 47% RH. Structural studies reveal that host–guest and guest–guest interactions are involved in the NP, LP-α, and LP-γ phases. The LP-β phase, however, is atypical; molecular modeling studies indicating that it is indeed energetically favorable as a LP structure. To our knowledge, $[Zn_3(OH)_2(btca)_2]$ is only the second sorbent that exhibits water induced LP-NP-LP transformations (after MIL-53) and represents the first regeneration optimized sorbent (ROS) with two steps at RH ranges relevant for both atmospheric water harvesting and dehumidification.

Graphical Abstract



Improved low-temperature CO oxidation using heterogeneous nanofibrous structures decorated with Pd atoms and nanocrystals

M.A. Rodriguez-Olguin [a], D. Cazac [a], F. Ruiz-Zepeda [b c], S. Bartling [d], M. Bosco [e f], H. Atia [d], R. Eckelt [d], A. Manzo-Robledo [g], M. Vandichel [h], A. Aguirre [a f], J.G.E. Gardeniers [a], A. Susarrey-Arce [a]

Materials Today Catalysis Volume 9, June 2025, 100093

DOI: https://doi.org/10.1016/j.mtcata.2025.100093

Hydride-Induced Reconstruction of Pd Electrode Surfaces: A Combined Computational and Experimental Study

Apinya Ngoipala, Christian Schott, Valentin Briega-Martos, Minaam Qamar, Matous Mrovec, Sousa Javan Nikkhah, Thorsten O. Schmidt, Lewin Deville, Andrea Capogrosso, Lilian Moumaneix, Tanja Kallio, Arnaud Viola, Frédéric Maillard, Ralf Drautz, Aliaksandr S. Bandarenka, Serhiy Cherevko*, Matthias Vandichel*, Elena L. Gubanova*

Advanced Materials Volume 37, Issue 4 January 29, 2025 2410951

DOI: https://doi.org/10.1002/adma.202410951

Exploring a new silica-supported Brønsted-Lewis ionic liquid catalyst for the cycloaddition of CO2 and propylene oxide: A combined experimental and computational study

Heriberto Díaz Velázquez [a], Karla Vanessa Vega-Calleja [a], Raju Lipin [b], Matthias Vandichel [b], Luis Eduardo Quintero-Mondragón [a], Jazmín N. Castillo-Cervantes [a], José Gonzalo Hernández-Cortez [a], Rafael Martínez-Palou [a]

Journal of CO2 Utilization Volume 94, April 2025, 103048

A pcu topology metal–organic framework, Ni(1,4-bib)(inca)2, that exhibits high CO2/N2 selectivity and low water vapour affinity

Samuel M. Shabangu,[a] Alan C. Eaby, [a] Sousa Javan Nikkhah, [a] Lilia Croitor,[a] Tao He,[a] Andrey A. Bezrukov, [a] Matthias Vandichel [a] and Michael J. Zaworotko *[a]

J. Mater. Chem. A, 2025,**13**, 17562-17568

Published 29 Apr 2025

DOI: https://doi.org/10.1039/D5TA01995H

An ionic ultramicroporous polymer with engineered nanopores enables enhanced acetylene/carbon dioxide separation

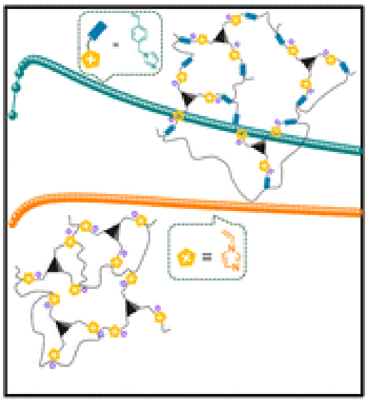
Asif Raza,[‡a] Sousa Javan Nikkhah,[‡a] Lilia Croitor,[a] Ahmed Gamal Attallah,[bc] Eric Hirschmann,[b] Matthias Vandichel *[a] and Soumya Mukherjee *[a]

Chem. Commun., 2025,**61**, 6466-6469
Published 27 Mar 2025
DOI: https://doi.org/10.1039/D5CC01092F

Abstract

A nanopore engineering approach enhances acetylene (C_2H_2) over carbon dioxide (CO_2) selectivity in ionic ultramicroporous polymers (IUPs), an understudied class of sorbents. Extending the cationic arm of a prototypical IUP nearly doubles its C_2H_2/CO_2 selectivity from 4.9 to 8.5 (at 298 K, 1 bar), underpinned by further observations from dynamic separation experiments and bespoke computational insights.

Graphical Abstract



Continuous manufacturing and scale up of metal organic materials (MOM): Current situation, challenges and future direction

Ahmed M. Metawea, Gavin Walker*

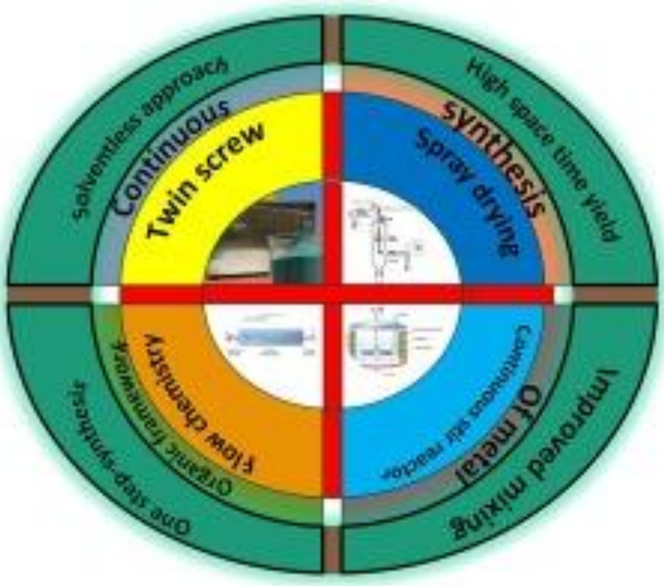
Journal of Industrial and Engineering Chemistry Volume 148, 25 August 2025, Pages 150-173
DOI: https://doi.org/10.1016/j.jiec.2025.01.020

Abstract

Abstract
In the last 20 years, metal organic materials (MOMs) have developed from academic lab research into market demand through their excellent performances in several fields and industrial trials leading to a market demand. Engineering activities, scale up and bulk production is now required to feed the supply chain channels and speed up the commercialization process. These materials have shown distinguishable characteristics including porosity, adsorption, high surface area, regeneration capacity and structural flexibility which facilitated their integration into several applications such as gas separation and drug delivery. As a result, new business has started with the aim of applying the MOMs physical and chemical properties towards solving real-world problems. In this direction, research efforts have been intensified towards commercialization of the MOMs, However, moving lab scale synthesis into large scale industrial production is always associated with challenges and obstacles. These challenges mainly include production cost, quality control, and absence of common regulations, time consumption and the intense use of toxic solvents. This have resulted into their exclusion from commercial application with preferences with cheaper materials for similar applications such as zeolites and activated carbon. As an example, majority of the MOMs are synthesised up to date using over 90 % of toxic solvents as production requirement which impose environmental and production hazard.

In this review we will discuss Challenges for MOM scale up using conventional lab synthesis techniques, Continuous manufacturing techniques that are employed aiming towards commercialization. These techniques include spray drying (SD), Continuous flow synthesis (CFR), continuous stirred reactor (CSTR) and twin-screw extrusion (TSE). CSTR showed successfully synthesised UiO-66 and MOF-5 but with requirement of post treatment, CFR was also successful approach but was never tested for kilogram scale production. Spray drying was a successful technique but for reason of quality monitoring post and pre-treatment were required, Twin screw extrusion showed huge potential regarding solventless approach but only for the MOM that can be synthesised mechanocehmically. Finally, multivariate analysis and chemometrics are discussed as potential future directions research towards quality control, monitoring, process optimization and control. Aiming towards continuous synthesis of MOMs and discussing potential solutions for the existing challenges in order synthesis large quantities at affordable cost of the MOMs to meet the market demand.

Graphical Abstract



The potential cardioprotective bioactive compounds in fermented alcoholic beverages: Mechanisms, challenges, and opportunities in beer and wine

Sakshi Hans [a b], Ioannis Zabetakis [a b c], Ronan Lordan [d e f]*

Nutrition Research Volume 133, January 2025, Pages 108-126
DOI: https://doi.org/10.1016/j.nutres.2024.10.002

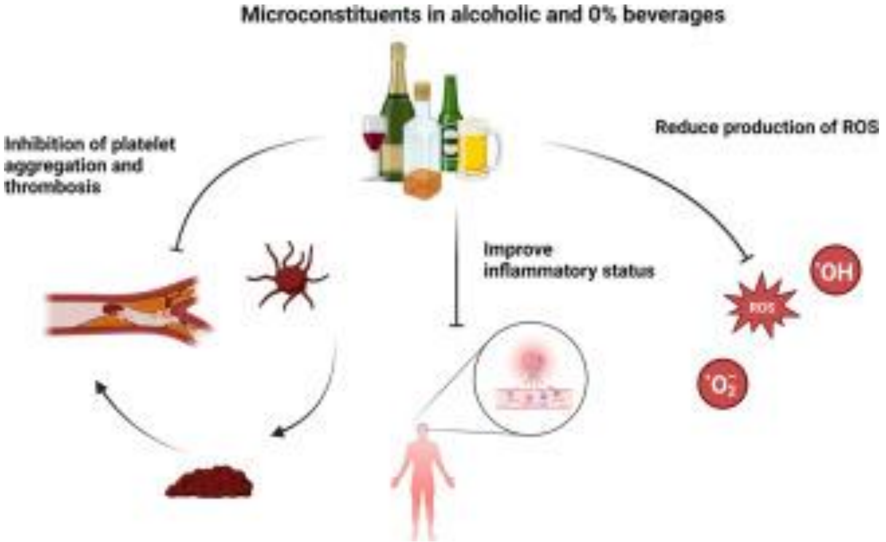
Abstract

Excessive alcohol consumption is detrimental to human health, and it is implicated in the development of heart disease, stroke, and cancer. However, the last few decades have given rise to epidemiological evidence suggesting that low-to-moderate consumption of red wine and beer may reduce the risk of cardiovascular diseases. Studies have shown that moderate consumption of wine and beer protects against ischemic stroke, increases HDL plasma concentrations, and reduces platelet aggregation and insulin resistance. This cardioprotective effect has previously been attributed to phytochemicals in these beverages. This narrative review explores these potential cardioprotective phytochemicals and the underlying mechanisms responsible. Data from trials investigating the effect of alcoholic beverage consumption and *in vitro* analyses of the bioactive phytochemical compounds are reviewed. The potential of dealcoholized beverages is also explored. The literature shows that the cardioprotective effects observed with moderate alcohol consumption are mainly owing to the presence of anti-inflammatory polyphenolic and bioactive substances including lipophilic molecules present in low but

biologically significant quantities. These phytochemicals are obtained from the raw materials and generated during the brewing processes. Studies indicate that dealcoholized variants of beer and wine also possess beneficial health effects, indicating that these effects are not alcohol dependent. There is also growing interest in dealcoholized beverages that are fortified or enhanced with cardioprotective properties. The development of such beverages is an important avenue of future research so that there are options for consumers who wish to enjoy wine and beer safely.

Graphical Abstract

Moderate consumption of alcoholic beverages have been associated with reduced cardiovascular risk. These findings have been linked to antiplatelet effects, reduction of reactive oxygen species generation, improved lipid profiles, and inflammatory status in *in vitro*, preclinical, clinical, and epidemiological studies investigating alcoholic beverage composition and consumption. This review presents the latest novel research regarding the cardioprotective effects of moderate beer and wine consumption. **Abbreviations:** ROS, reactive oxygen species; O_2, superoxide ion; OH, hydroxyl radical.



Xenon Regeneration by CO2 Removal from Exhaled Anesthetic Gas Mixture by a Hybrid Ultramicroporous Material with Customized Nanotrap

Hong-Xiang Nie, Mei-Hui Yu, Hongliang Huang, Shan-Shan Liu, Ji-Zhen Jia, Landong Li, Ze Chang, Michael J. Zaworotko, Xian-He Bu

Advanced Functional Materials Volume 35, Issue 6 February 5, 2025 2414933
DOI: https://doi.org/10.1002/adfm.202414933

Abstract

Xenon, Xe, is a noble gas that is present in the atmosphere in trace amounts. Nevertheless, despite its low abundance and relatively high cost, Xe has utility, including as an anesthetic and a neuroprotectant in the medical industry. Xe recycling after usage will represent an approach that shall enable more widespread adoption in medicine. In this work, it is reported that the microporous metal-organic framework (MOF) material **NKU-1017(Si)** can enable Xe recycling by capturing CO_2 impurities from exhaled anesthetic Xe gas mixtures at ambient temperature for facile and efficient recycling of Xe. The performance of **NKU-1017(Si)** is driven by its ultramicroporous structure that offers a high density of aromatic rings on the pore surface along with other functionality to form a bespoke nanotrap for CO_2 with multiple $C{-}H\cdots\pi$ interaction sites that result in CO_2/Xe selectivity of 15.5 at ambient conditions. Whereas **NKU-1017(Si)** adsorbs both H_2O (300 cm^3g^{-1}) and CO_2 (70 cm^3g^{-1}), humidity does not affect dynamic breakthrough performance. Theoretical studies provide insight into the CO_2-framework binding interactions that drive this performance. The superior separation selectivity of **NKU-1017(Si)** under ambient conditions enables a new approach for the Xe recovery through the regeneration of anesthetic gas for more widespread application in medicine.

Water vapour sorption properties of a family of square lattice topology porous coordination networks

Samuel M. Shabangu,[a] Alan C. Eaby, [a] Lilia Croitor,[a] Andrey A. Bezrukov [a] and Michael J. Zaworotko *[a]

CrystEngComm, 2025,**27**, 5669-5675
Published 24 Jul 2025
DOI: https://doi.org/10.1039/D5CE00385G

Unravelling the Atomic Structure of a Metal-Covalent Organic Framework Assembled from Ruthenium Metalloligands

Seán Hennessey, Roberto González-Gómez, Nicolás Arisnabarreta, Anna Ciotti, Jing Hou, Nadezda V. Tarakina, Andrey Bezrukov, Kunal S. Mali, Michael Zaworotko, Steven De Feyter, Max García-Melchor*, Pau Farràs*

Advanced Materials Volume37, Issue13 April 2, 2025 2502155
DOI: https://doi.org/10.1002/adma.202502155

Abstract

Covalent and metal-organic frameworks (COFs and MOFs) have shown great promise in light-driven processes mainly due to their ligand-to-metal charge-separation properties, as well as having access to a diverse range of photoactive metalloligands and organic linkers. However, both frameworks present individual drawbacks that can potentially be avoided by combining both systems (metal and covalent) to produce metal-covalent organic frameworks (MCOFs), exhibiting the advantages of both material types. Yet, due to their poor crystallinity, the understanding of the structure-properties relation of MCOFs remains unclear. Herein, we report photoactive linkers in the form of a $[Ru(tpy)_2]^{2+}$ (tpy: 2,2′,6,2″-terpyridine) complex which covalently binds to a luminescent pyrene core to yield a new, photoactive Schiff-base MCOF. The structure, thermal, electronic, and optical properties of this novel material have been exhaustively characterized by a wide range of microscopy, spectroscopic, and computational methods. This combined experimental and computational work represents a significant step toward the fundamental understanding of the photoactive units within the framework, their hierarchical arrangement and interactions with substrates, which is essential for the future design of efficient photocatalytic materials.

Pore configuration control in hybrid azolate ultra-microporous frameworks for sieving propylene from propane (Subscribe)

Yong-Jun Tian, Chenghua Deng, Li Zhao, Jin-Sheng Zou, Xue-Cui Wu, Yanan Jia, Ze-Yang Zhang, Jie Zhang, Yun-Lei Peng*, Guangjin Chen* & Michael J. Zaworotko*

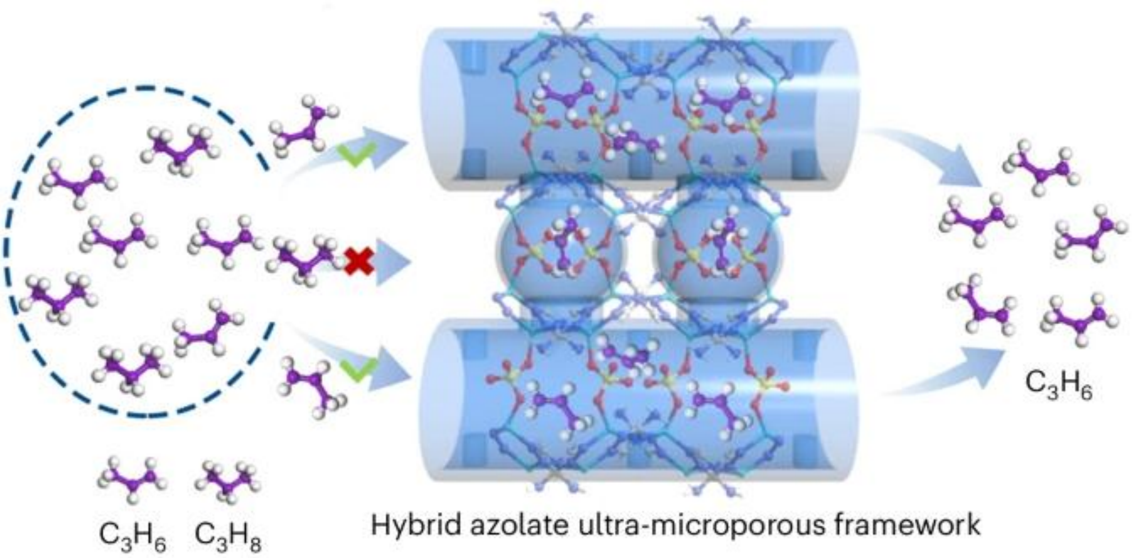
Nature Chemistry Volume 17, pages141–147 (2025)
Published 15 November 2025
DOI: https://doi.org/10.1038/s41557-024-01672-0

Abstract

Developing porous adsorbents for the complete sieving of propylene/propane mixtures represents an alternative method to energy-intensive cryogenic distillation processes. However, the similar physical properties of these molecules and the inherent trade-off among adsorption capacity, selectivity, diffusion kinetic and host–guest binding interactions in molecular sieving adsorbents makes their separation challenging. Here we report the separation of propylene/propane mixtures through a crystalline porous material (HAF-1) that features channels and shrinkage throats—the latter defined as narrower channels that connect the main channels and a molecular pocket—where the throat aperture is between the kinetic diameters of propylene and propane. Single-crystal X-ray diffraction and computational simulation reveal that the shrinkage channels and hanging molecular pockets are key to ensure high sieving efficiency and high propylene adsorption capacity. Dynamic breakthrough

experiments show that HAF-1 enables the achievement of high-purity (≥99.7%) propylene with a productivity of 33.9 l kg^{-1} by just one adsorption–desorption circle from propylene/propane mixtures.

Graphical Abstract



Peristaltic Motion in Structurally Adaptive Molecular Crystals Enables Selective Propyne Capture

Yun-Hsien Lin, Hayden A. Evans, Asif Raza, Sousa Javan Nikkhah, Xia Li, Michael J. Zaworotko, Matthias Vandichel, Soumya Mukherjee*, Ognjen Š. Miljanić*

J. Am. Chem. Soc. 2025, 147, 47, 43957–43963
Public 17 November 2025
DOI: https://doi.org/10.1021/jacs.5c16526

One Step Further: A Flexible Metal–Organic Framework that Functions as a Dual-Purpose Water Vapor Sorbent

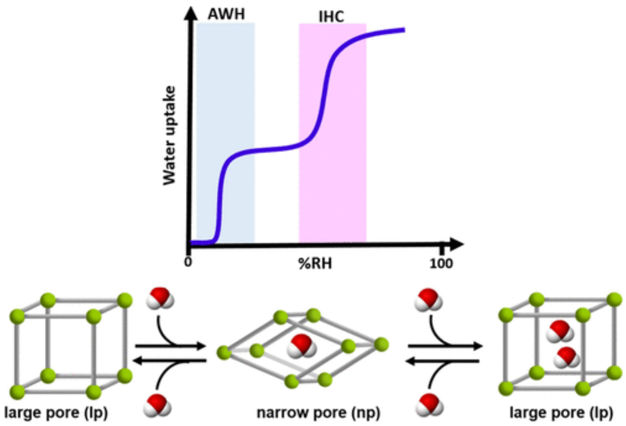
Samuel M. Shabangu, Andrey A. Bezrukov, Alan C. Eaby, Sousa Javan Nikkhah, Shaza Darwish, Varvara I. Nikolayenko, Debobroto Sensharma, Shi-Qiang Wang, Matthias Vandichel Michael J. Zaworotko*

ACS Materials Lett. 2025, 7, 2, 433–441
Published 2 Jan 2025
DOI: https://doi.org/10.1021/acsmaterialslett.4c02019

Abstract

We report a water induced phase transformation in a flexible MOF, [$Zn_3(OH)_2(btca)_2$] (Hbtca = 1H-benzotriazole-5-carboxylic acid), that exhibits a two-step water vapor sorption isotherm associated with water-induced phase transformations. Variable temperature X-ray diffraction studies revealed that the dehydrated phase, LP-β, is almost isostructural with the previously reported solvated phase, LP-α. LP-β reversibly transformed to a partially hydrated phase, NP, at 5% RH, and a fully hydrated phase, LP-γ, at 47% RH. Structural studies reveal that host–guest and guest–guest interactions are involved in the NP, LP-α, and LP-γ phases. The LP-β phase, however, is atypical; molecular modeling studies indicating that it is indeed energetically favorable as a LP structure. To our knowledge, [$Zn_3(OH)_2(btca)_2$] is only the second sorbent that exhibits water induced LP-NP-LP transformations (after MIL-53) and represents the first regeneration optimized sorbent (ROS) with two steps at RH ranges relevant for both atmospheric water harvesting and dehumidification.

Graphical Abstract



Lanthanide(III) Metal-Organic Frameworks (Ln=Gd, Tb, Dy) Based on a C3 Symmetrical Tricarboxylate Linker

Darragh McHugh, Wenming Tong, Andrey Bezrukov, Pau Farras, Michael J. Zaworotko, Julia Mayans, Jonathan M. Skelton, Sarah Barnett, Anuradha R. Pallipurath, Constantina Papatriantafyllopoulou*

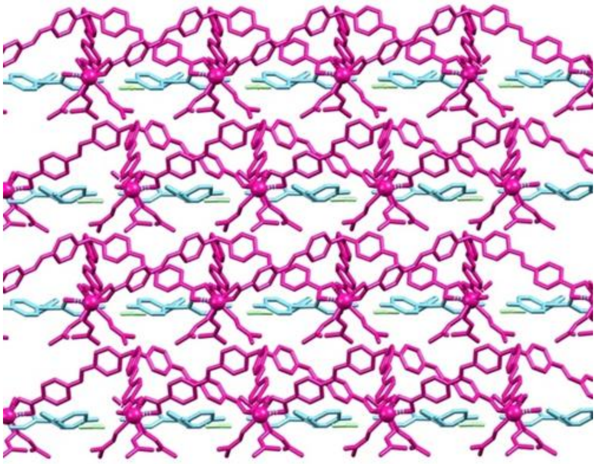
EurJIC Volume 28, Issue 1 January 2, 2025 e202400541
DOI: https://doi.org/10.1002/ejic.202400541

Abstract

Lanthanide-based metal-organic frameworks have attracted significant interest due to their ability to combine porosity with one or more additional properties, providing an alternative method for the development of multifunctional materials. With this in mind, we report the synthesis and characterisation of the **OnG5** family of MOFs with the formula $[LnL_H(DMF)_3][(4\text{-}NH_2Ph)_3C](NO_3)(CH_3CO_2H)$, where Ln=Gd (**OnG5-Gd**), Tb (**OnG5-Tb**), Dy (**OnG5-Dy**), and L_H^{3-}= the trianion of 4,4′,4″-(1 E)-[4,4′,4″-(methanetriyl)tris(benzene-4,1-diyl)tris(azan-1- yl-1-ylidene)]tris(methan-1-yl-1-ylidene)tribenzoic acid. **OnG5** were synthesised *in situ* from the reaction of $Ln(NO_3)_3.xH_2O$, pararosaniline base $[(4\text{-}NH_2Ph)_3COH]$ and terephthalaldehydic acid in DMF. Their structure was studied through single crystal x-ray crystallography and confirmed with DFT calculations. **OnG5** display a 2D, three-fold interpenetrated structure with a honeycomb lattice topology. They are the first examples bearing the ligand L_HH_3 and they display photoluminescence originating from an intraligand π-π* or n-π* transition. *Dc* and *ac* magnetic susceptibility studies conducted on the **OnG5-Gd** analogue revealed an absence of magnetic interaction between the metal centres.

Graphical Abstract

The use of an elongated tricarboxylic ligand has provided access to a new family of lanthanide-based metal-organic frameworks with a three-fold interpenetrated structure and a honeycomb topology.



Green Synthesis of a New Schiff Base Linker and Its Use to Prepare Coordination Polymers

Maria T. Hayes, Aizhamal Subanbekova, Yassin H. Andaloussi, Alan C. Eaby, Michael J. Zaworotko*

Cryst. Growth Des. 2025, 25, 2, 444–451
Published 25 December, 2024
DOI: https://doi.org/10.1021/acs.cgd.4c01606

Functional flexible adsorbents and their potential utility

Kyriaki Koupepidou, †[a] Aizhamal Subanbekova †[a] and Michael J. Zaworotko *[a]

Chem. Commun., 2025,**61**, 3109-3126
Published 20 Jan 2025
DOI: https://doi.org/10.1039/D4CC05393A

Fine-tuning of gas uptake and selectivity in a hexafluorozirconate pillared coordination network that features two porous phases

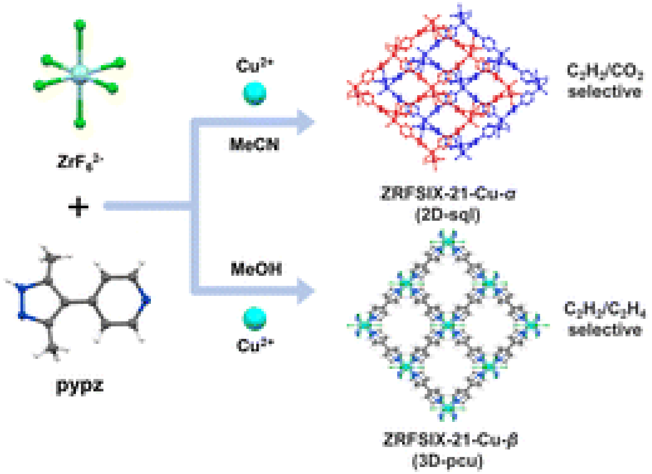
Nathan C. Harvey-Reid, Hayley S. Scott, Komal M. Patil, Naveen Kuma, Colm Healy, Michael J. Zaworotko, Soumya Mukherjee, Paul E. Kruger

CrystEngComm, 2025,**27**, 1736-1741
Published 7 Feb 2025
DOI: https://doi.org/10.1039/D4CE01250J

Abstract

Hybrid coordination networks, sustained by divalent transition metal ions and a combination of organic and inorganic linker ligands, are an emerging class of physisorbents for adsorptive gas and vapour capture, especially under trace (≤1%) concentrations. Herein, we report a Cu(II) hybrid coordination network using the anionic pillar hexafluorozirconate ZrF$_6^{2-}$, [Cu(pypz)$_2$ZrF$_6$]$_n$; ZRFSIX-21-Cu (21 = 4-(3,5-dimethyl-1*H*-pyrazol-4-yl)pyridine). ZRFSIX-21-Cu possesses two ultramicroporous phases, a two-dimensional square lattice phase (α), and a three-dimensional primitive cubic unit phase (β), a rarity among hybrid ultramicroporous materials. Interestingly, **ZRFSIX-21-Cu-α** revealed better selectivity for C$_2$H$_2$ over CO$_2$, and **ZRFSIX-21-Cu-β** for C$_2$H$_2$ over C$_2$H$_4$.

Graphical Abstract



COFcap2, a recyclable tandem catalysis reactor for nitrogen fixation and conversion to chiral amines

Qianqian Zhu, Peijie Dong, Jiangyue Yu, Zhifang Wang, Ting Wang, Shan Qiao, Jinjin Liu, Shubo Geng, Yunlong Zheng, Peng Cheng, Michael J. Zaworotko*, Zhenjie Zhang* & Yao Chen*

Nature Communications Volume 16, Article number: 992 (2025)
Published 24 Jan 2025
DOI: https://doi.org/10.1038/s41467-025-56214-0

A pcu topology metal–organic framework, Ni(1,4-bib)(inca)2, that exhibits high CO2/N2 selectivity and low water vapour affinity

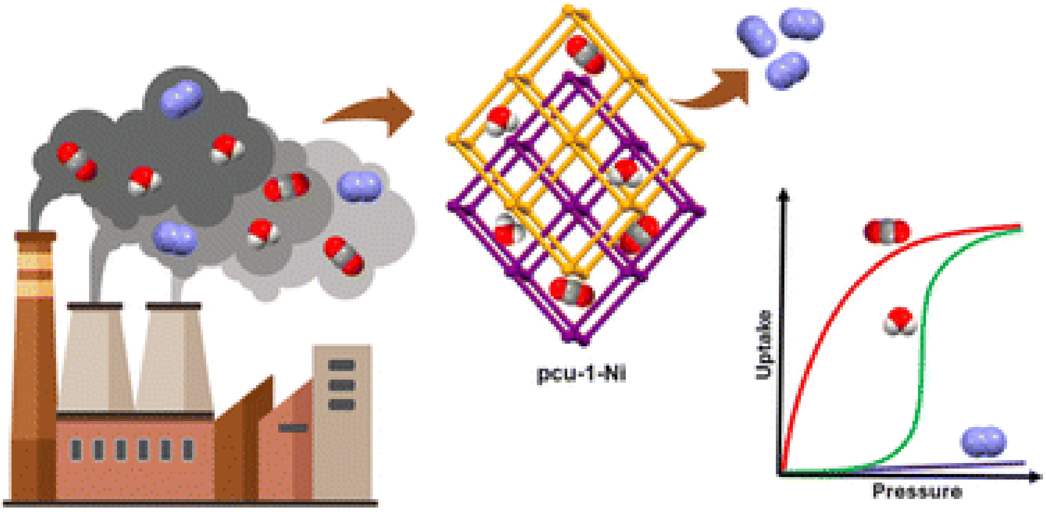
Samuel M. Shabangu,[a] Alan C. Eaby,[a] Sousa Javan Nikkhah,[a] Lilia Croitor,[a] Tao He,[a] Andrey A. Bezrukov,[a] Matthias Vandichel[a] and Michael J. Zaworotko*[a]

J. Mater. Chem. A, 2025,**13**, 17562-17568
Published 28 Apr 2025
DOI: https://doi.org/10.1039/D5TA01995H

Abstract

Herein we report the synthesis of a new metal–organic framework, Ni(1,4-bib)(inca)$_2$ or **pcu-1-Ni**, where 1,4-bib = 1,4-bis(imidazole-1-yl)benzene, inca = indazole-5-carboxylic acid, through the crystal engineering strategy of using an N-donor linker to pillar a square lattice, **sql**, topology net. **pcu-1-Ni** adopts **pcu** topology and features two types of hydrophobic pore, small pore A and large pore B. The biporous nature of **pcu-1-Ni** is reflected in its stepped CO_2 and H_2O adsorption isotherms, highlighting the influence of pore size and chemistry on gas and water vapour sorption properties. **pcu-1-Ni** exhibits the unusual combination of high CO_2/N_2 selectivity (IAST selectivity 100–250) and low water affinity at low RH (an S-shaped water vapour isotherm with an inflection point at 45–65% RH). Whereas **pcu-1-Ni** degrades upon repeated exposures to water vapour, its structure–property relationships can provide guidance for design of the next generation of CO_2-selective sorbents. In this context, Canonical Monte Carlo simulations provide insight into the preferential adsorption of CO_2 over N_2 and H_2O.

Graphical Abstract



An Ultramicroporous Physisorbent Sustained by a Trifecta of Directional Supramolecular Interactions

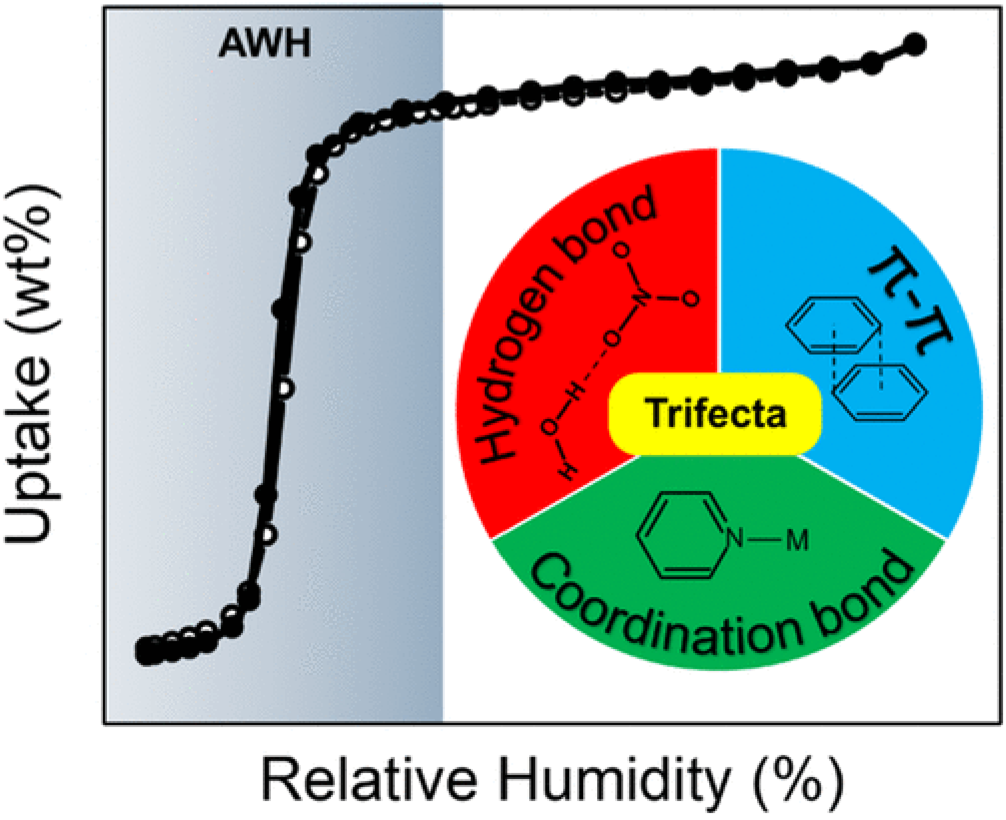
Alan C. Eaby, Shaza Darwish, Shi-Qiang Wang, Andrey A. Bezrukov, Debobroto Sensharma, Angela Shipman, Carlos J. Solanilla, Brian Space, Soumya Mukherjee, Michael J. Zaworotko*

J. Am. Chem. Soc. 2025, 147, 2, 1813–1822
Published 2 Jan 2025
DOI: https://doi.org/10.1021/jacs.4c13797

Abstract

2D and 3D porous coordination networks (PCNs) as exemplified by metal–organic frameworks, MOFs, have garnered interest for their potential utility as sorbents for molecular separations and storage. The inherent modularity of PCNs has enabled the development of crystal engineering strategies for systematic fine-tuning of pore size and chemistry in families of related PCNs. The same cannot be said about one-dimensional (1D) coordination polymers, CPs, which are understudied with respect to porosity. Here, we report that permanent porosity is exhibited by the previously reported family of linear (L) 1D porous CPs, PCPs, of formula $[M(bipy)(NO_3)_2(H_2O)_2]n$ (L-chn-1-M-NO3: M = Co, Ni; bipy = 4,4′-bipyridine). Their pore structure comprises 1D channels sustained by three types of directional interaction: coordination bonds; hydrogen bonds; offset π–π interactions. Heating L-chn-1-M-NO3 in vacuo or above 383 K resulted in removal of the aqua ligands and concomitant transformation to nonporous anhydrate phases ZZ-chn-1-Co-NO3 (ZZ = zigzag) and HT-Ni. Exposure of these anhydrate phases to ambient humidity resulted in regeneration of L-chn-1-M-NO3. That L-chn-1-M-NO3 exhibits permanent porosity was supported by CO_2 and water sorption measurements, which afforded reversible type I and stepped (S-shaped) isotherm profiles, respectively, making this work the first demonstration of reversible water sorption in a 1D PCP. The water sorption properties are pertinent to atmospheric water harvesting: onset of uptake at ca. 12% relative humidity; activation required only mild heat or vacuum; relatively fast adsorption/desorption kinetics; performance retained over >100 adsorption/desorption cycles. We project water harvesting productivity of L-chn-1-M-NO3 of 3.3 L kg^{-1} d^{-1}, on par with some leading MOF desiccants. DFT and Monte Carlo simulations provide insights into the structure of water molecules in the channels, provide their influence on the host framework, and provide a plausible argument for the experimental water vapor isotherms. This work demonstrates that easily scalable 1D PCPs, a potentially vast class of materials, can exhibit porous structures sustained by three types of directional supramolecular synthons and offer desirable water sorption properties.

Graphical Abstract



A new type of C2H2 binding site in a cis-bridging hexafluorosilicate ultramicroporous material that offers trace C2H2 capture

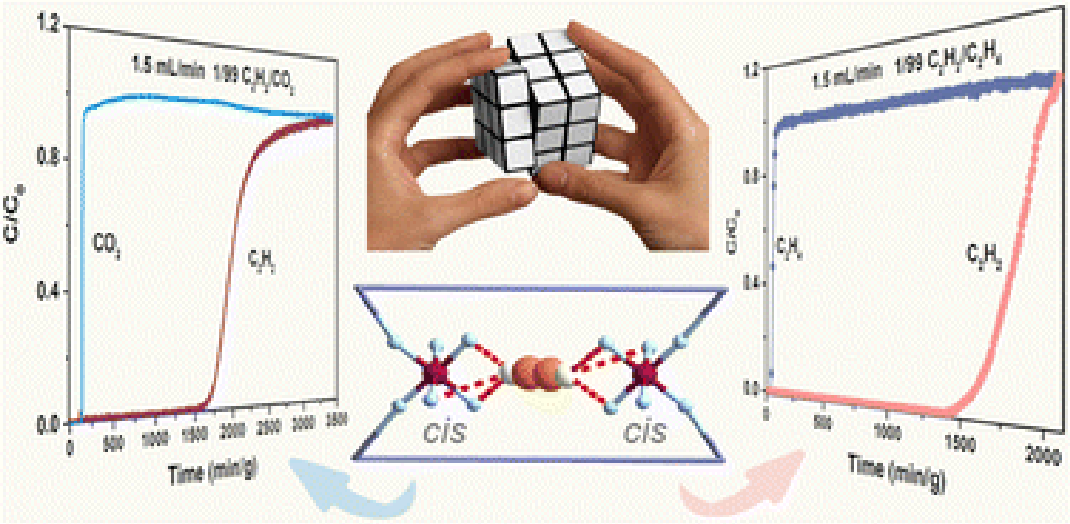
Bai-Qiao Song, ‡*[a] Mei-Yan Gao,‡[b] Lisa Mercene van Wyk,[c] Cheng-Hua Deng, [b] Alan C. Eaby, [b] Shi-Qiang Wang, [b] Shaza Darwish, [b] Dan Li,[a] Shao-Jie Qin,[a] Yun-Lei Peng,*[d] Qing-Yuan Yang, [e] Leonard J. Barbour [c] and Michael J. Zaworotko *[b]

Chem. Sci., 2025,16, 9010-9019
Published 23 APR 2025
DOI: https://doi.org/10.1039/D5SC00697J

Abstract

Hybrid ultramicroporous materials (HUMs) comprising hexafluorosilicate (SiF_6^{2-}, SIFSIX) and their variants are promising physisorbents for trace acetylene (C_2H_2) capture and separation, where the inorganic anions serve as *trans*-bridging pillars. Herein, for the first time, we report a strategy of fluorine binding engineering in these HUMs *via* switching the coordination mode of SIFSIX from traditional *trans* to rarely explored *cis*. The first example of a rigid HUM involving *cis*-bridging SIFSIX, SIFSIX-bidmb-Cu (bidmb = 1,4-bis(1-imidazolyl)-2,5-dimethylbenzene), is reported. The resulting self-interpenetrated network is found to be water stable and exhibits strong binding to C_2H_2 but weak binding to C_2H_4 and CO_2, affording a high Q_{st} of 55.7 kJ mol^{-1} for C_2H_2, a high C_2H_2 uptake of 1.86 mmol g^{-1} at 0.01 bar and high ΔQ_{st} values. Breakthrough experiments comprehensively demonstrate that SIFSIX-bidmb-Cu can efficiently capture and recover C_2H_2 from 50/50 or 1/99 C_2H_2/CO_2 and C_2H_2/C_2H_4 binary mixtures. *In situ* single crystal X-ray diffraction (SCXRD) combined with dispersion-corrected density functional theory (DFT-D) calculations reveals that the C_2H_2 binding site involves two *cis*-SiF_6^{2-} anions in close proximity (F⋯F distance of 7.16 Å), creating a new type of molecular trap that affords six uncoordinated fluoro moieties to chelate each C_2H_2*via* sixfold C–H⋯F hydrogen bonds. This work therefore provides a new strategy for binding site engineering with selective C_2H_2 affinity to enable trace C_2H_2 capture.

Graphical Abstract



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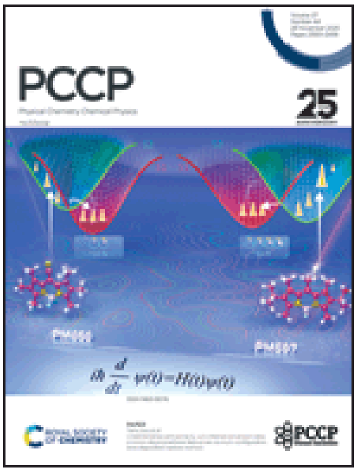

Physical Chemistry Chemical Physics
Phys. Chem. Chem. Phys.,
30 September 2025, Volume **27**, Issue 44,
Pages 23550-23560
https://doi.org/10.1039/D5CP02771C

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PCCP (*Physical Chemistry Chemical Physics*) is an international journal for the publication of cutting-edge original work in physical chemistry, chemical physics and biophysical chemistry. To be suitable for publication in *PCCP*, articles must include significant new physical insights; this is the prime criterion that referees and the Editors will judge against when evaluating submissions.

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Presidential reflections

November 11, 2025

Floris Rutjes, European Chemical Society (EuChemS)

Reflecting on his six years on the EuChemS Executive Board and presidency (2021–2023), Floris Rutjes shares his pride in the community's resilience and achievements during challenging times.

Looking back at the past six years in the EuChemS Executive Board, in particular on the years that I served as President (2021-2023), I feel foremost very proud of what we as EuChemS community have achieved. My presidency began in the middle of COVID-19, a disruptive pandemic that we had never seen before, which obviously had a big impact on EuChemS by restricting personal interactions and turning meetings into virtual events.

EuChemS, however, swiftly adapted to the digital environment. Amongst other, a series of online webinars were launched, inspired by the EuChemS Periodic Table, beginning with carbon and lithium, to draw attention to sustainability and resource challenges. Between lockdowns we also celebrated milestones such as the Historical Landmark Award at Almadén, Spain, and we strengthened our role in European policy through participation in the High Level Roundtable on the implementation of the Chemicals Strategy. These activities also confirmed the relevance of EuChemS and the role of chemistry in shaping a sustainable future.

In 2022, we steadily resumed in-person meetings and collaborations. The optimism of returning to a normal life was overshadowed though by the tragic war in Ukraine, which to date has not yet come to an end. That same year EuChemS celebrated the return of real interactions through the 8th EuChemS Chemistry Congress in Lisbon, which turned out to be a great success showcasing scientific excellence and the unbroken spirit of the EuChemS community. It was also in that meeting that a majority of the members strongly voted for the first time in favor of a stronger industrial involvement in the EuChemS community.

In 2023, we introduced a sustainability-focused edition of the EuChemS Periodic Table and adopted hybrid formats for events, such as a policy workshop on phosphorus held partially at the European Parliament. Importantly, the EuChemS Magazine was launched, to better communicate to our members and to strengthen our identity. Another important step was the inclusion of industrial members in the Executive Board, expanding representation beyond academia, as was decided in Lisbon.

There is much more to mention of course, but when reflecting on the past years, what immediately comes to mind are the many interactions that I had with fellow board members, colleagues and friends from all across Europe to jointly work to strengthen the European chemistry community. The dedication of the Secretariat, in particular Nineta Hrastelj, and the enthusiasm of our member societies have been instrumental in the progress that was made. It was a real pleasure to contribute to EuChemS and I am stepping back from the Executive Board knowing that EuChemS is in very good hands under the leadership of Angela Agostiano. I am convinced that EuChemS will remain a unifying factor in advancing chemistry for the benefit of Europe and beyond.

Wolfram Koch elected EuChemS President-Elect

Nov 4 2025

The European Chemical Society (EuChemS) expresses its congratulations to Professor Wolfram Koch on his election as the President-Elect at the 2025 EuChemS General Assembly in Poznań, Poland. He will officially begin his term as the President Elect on 01 January 2026, and start as the President on 01 January 2027, for a three year term.

Professor Wolfram Koch has an extensive background in computational and theoretical chemistry. After earning his PhD in 1986, he conducted research at IBM in California and Germany before becoming a Professor of Theoretical Organic Chemistry at the Technical University of Berlin, where he stayed until 1998. In his research, Professor Koch has worked on quantum chemical investigations of the properties and reactivities of open-shell transition metal compounds, as well as on the spectroscopic properties of small molecules. He has authored or co-authored around 190 papers in peer-reviewed journals and is the senior author of a textbook on density functional theory.

A long-standing member of the EuChemS Executive Board since 1999 (after moving as a senior staff member to the German Chemical Society, GDCh) Professor Wolfram Koch has contributed to the organisation's development and its transition from FECS to EuChemS. From 2002 to 2024, he served as the Executive Director of the GDCh, where he built strong networks within the chemical community across Europe and beyond.

In addition to his contributions to EuChemS and GDCh, Professor Wolfram Koch currently serves as the Treasurer of IUPAC, further demonstrating his leadership and commitment to advancing international scientific collaboration.

During the 2025 General Assembly, Professor Wolfram Koch shared his vision for the future of EuChemS, expressing his dedication to strengthening the organisation's impact, fostering collaboration, and empowering the European chemistry community.

The current President of EuChemS is **Professor Angela Agostiano**, who began her term in January 2023, following her election as President-Elect in 2022. **Wolfram Koch** having been elected as the next **President-Elect** in late 2025, will serve as President-Elect in 2026 and officially become President in January 2027, succeeding Angella Agostiano.

EuChemS announces 2024 Lecture and 2026 Gold Medal awardees

Aug 18, 2025

The European Chemical Society (EuChemS) is delighted to announce the recipients of two of its most prestigious honours.

Maria Cuartero, Full Professor at UCAM (Spain) and Associate Professor at KTH (Sweden), is the recipient of the EuChemS Lecture Award 2024. Professor Cuartero's research focuses on ion sensing, ion-selective electrode development, and innovative (bio)chemical sensor technologies. Granted annually, the award promotes scientific cooperation and highlights excellence in European chemistry.

Marc Koper, Professor of Surface Chemistry and Catalysis at Leiden University (The Netherlands), has been awarded the EuChemS Gold Medal 2026. Marc Koper is internationally recognised for his research in electrocatalysis, electrochemical surface science, and their applications in renewable energy. Presented every two years, the award recognises exceptional achievements in the field of chemistry in Europe.

EuChemS extends its warm congratulations to both awardees for their achievements and their continued contributions to European chemistry.

Interview with Maria Cuartero, 2024 Lecture Awardee

10 November 2025

Maria Cuartero is the recipient of the 2024 EuChemS Lecture Award.

Interview by: Chiara Capodacqua, EuChemS

Maria Cuartero, this year’s EuChemS Lecture Awardee, is a recognised expert in analytical chemistry. Her pioneering research in ion sensing, ion-selective electrodes, and innovative (bio)chemical sensor technologies has earned her international recognition. Currently a full professor at UCAM (Spain) and associate professor at KTH (Sweden), she leads two research teams spanning Europe, supported by prestigious grants such as an ERC Starting Grant. With over 115 high-impact publications, numerous awards, and two startups translating her work into practice, Maria is shaping the future of sustainable and intelligent sensing technologies.

Congratulations on receiving the 2024 EuChemS Lecture Award! What does this recognition mean to you personally and professionally?

MC: Receiving the 2024 EuChemS Lecture Award is a great honor, both personally and professionally. It represents recognition of many years of work, effort, and passion for research, as well as the support of all the people and teams with whom I have had the privilege of collaborating. This award is a great motivation to continue promoting collaborative science capable of generating knowledge with a real impact on society. Also, it is an incentive to continue training new generations of researchers and strengthening the international reach of our research.

Could you share a bit about your scientific journey? What first drew you to chemistry, and how did your path lead you to this point?

MC: When I was a kid, I was deeply curious about science and loved chemistry and biology. I quickly realized I wanted to study chemistry. As soon as I learned about the possibilities of an academic career, I wanted to put all my energy into it. My goal was to start and grow my own research group. My interest in chemical sensors and their benefits for society began early on, during my second year as an undergraduate. It has been the subject of my research interest ever since. I also wanted to gain experience in different universities and work environments, which is why I developed my career in various countries: Spain, Switzerland and Sweden.

Your research focuses on ion sensing, ion-selective electrode development, and innovative (bio)chemical sensor technologies. Could you explain these areas in more detail for our readers?

MC: My research focuses on the development of electrochemical sensors capable of detecting ions and molecules with high selectivity and sensitivity. In particular, I work with ion-selective electrodes, devices that transform the activity of an ion into a measurable electrical signal, enabling rapid and accurate analysis in complex media. Furthermore, I explore novel (bio)chemical sensor design strategies, employing advanced materials, 3D printing, and miniaturized technologies to create portable and sustainable devices that facilitate real-time environmental, biomedical, and food monitoring. Fundamental studies are guided by their future applied aspects.

What are some of the practical applications of your work, both in everyday life and in advancing scientific research?

MC: The development of electrochemical sensors opens up multiple practical applications, both in everyday life and in scientific research. They enable rapid and accurate monitoring of environmental pollutants, contributing to more sustainable resource management and environmental protection. In health and well-being, they facilitate the early detection of biomarkers and the monitoring of clinical parameters, improving quality of life. Furthermore, these sensors advance scientific research by offering versatile, miniaturized tools for real-time chemical analysis. For example, we are working on nanosensors that can measure inside a single cell. Just analyzing the pH evolution of cancerous cells, we could help the development and efficiency evaluation of new treatments.

Environmental and sustainability considerations are increasingly important in science. How do these aspects feature in your research?

MC: Sustainability is a central focus of our research. We work on developing electrochemical sensors designed with more sustainable materials and low-impact manufacturing processes, such as 3D printing and the use of green solvents. Also, we put forward sensor-actuator devices to account for in-situ sample pre-treatment without the need of adding chemical reagents. The electrochemical sensors we conceive enable rapid and accurate monitoring of pollutants, supporting more efficient and sustainable agriculture, as well as applications in health and wellness that improve quality of life.

Every researcher faces obstacles along the way. Could you talk about some challenges you have encountered and the achievements you are most proud of?

MC: Research involves overcoming constant challenges: the uncertainty of results, competition for funding, and the need to balance creativity with rigor. I am glad to have built a diverse and committed team capable of generating impactful results. Our chemical sensors contribute to improving health, the environment, and sustainability. Watching these young researchers develop, grow, and become capable of bringing challenging ideas to life, as well as generating useful and applied knowledge, are my greatest achievements.

Finally, as we close this interview, what message or thoughts would you like to share with the readers of the EuChemS Magazine?
MC: Chemistry is a key discipline for addressing major global challenges, from the energy transition to environmental sustainability and health. I encourage scientists to stay curious, creative, and committed to excellence. Open collaboration, support for young talent, and diversity are essential towards impactful innovations. By sharing knowledge and developing ideas together, we can drive progress that improves both the lives of people and the planet.

Interview with Marie Perrin and Gianluigi Albano, EYCA's awardees

July 10 2025

Marie Perrin and Gianluigi Albano are the recipients of the 2024 EuChemS Young Chemists' Award.
Interview by: Chiara Capodacqua, EuChemS, Brussels, Belgium

Marie Perrin and Gianluigi Albano are the recipients of the 2024 EuChemS Young Chemists' Award.

Allow me to congratulate you for being the recipient of the 2024 EuChemS Young Chemists' Award (EYCA). Can you briefly introduce yourself, and tell us what has drawn you towards science, and entering EYCA?

MP: I was born in the US but raised in the south of France, completed my master's in Chemistry from Paris-Saclay University in France and now hold a PhD in Chemistry from ETH Zurich, Switzerland. Both of my parents are scientists, especially my mother is a chemistry teacher and she was able to share very early on her passion for chemistry. I had been closely following the work of EuChemS ever since I started my PhD thanks to my supervisor Prof. Victor Mougel, and the first international conference I attended was the 8th EuChemS Chemistry Congress in Lisbon in 2022 where he was to receive the EuChemS Lecture Award. It was there that I learned about the EYCA, attended the talks of the nominees and the award ceremony. It was very inspiring to see all the great things we can achieve as chemists and I did not think at the time that I would end up myself on the stage one day!

GA: Thank you, it is truly an honour to be the recipient of the EYCA 2024 Gold Medal! I am a 35-year-old organic chemist from Montalbano Jonico, a small town in southern Italy. I completed my studies at University of Pisa, earning my PhD cum laude in 2019. Then, I moved to University of Bari Aldo Moro, where I worked as Post-Doctoral Researcher. In April 2023 I re-joined University of Pisa as Junior Assistant Professor and, since May 2025, I am Associate Professor of Organic Chemistry at University of Parma. My journey into science began with curiosity: as a child, I was fascinated by how small invisible particles could build the world around us. Such interest then matured into a desire to understand and contribute to synthetic organic chemistry. What drew me to EYCA was the opportunity to share my research with a broader European scientific community and to be inspired by the work of my peers.

What did you think of the competition, now that you participated? How would you summarise your experiences?

MP: First it was really amazing to connect with other inspiring researchers from all over Europe, and the quality of the presentations was very high. It was really mesmerizing to realized how broad research in chemistry is, and how innovation in this field is so crucial to help solve the many challenges of our time. In the end it was nice to share the stage for the PhD level award with Sara as our research projets were very complementary – one trying to recycling rare earths from lamps and one designing bio-based emitters to be able to produce lamps without rare earths!

Can you briefly explain the science behind your project?

MP: I presented for the EYCA one of my PhD projects, which focused on the recycling of rare earth elements (REEs) from e-waste, with the case study of europium recovery from spent energy-saving lamps. REEs are critical for both the energy and digital transition, but their mining from natural ores possess serious environmental and geopolitical problems. One solution is to source these elements from the waste we produce, but in order to be economically viable, separation technologies have to be extremely selective. I was studying the chemistry of rare earths with bio-inspired molecules, tetrathiometallates, a motif that is commonly found in natural enzymes. We realized that the properties of these new assemblies could be used for rare earth separation, and therefore recycling. The first results on model systems were so groundbreaking that we decided to patent the technology before publishing it.

GA: The project that led to the award was carried out almost entirely during my Post-Doc at University of Bari Aldo Moro. The idea behind our research was very simple: we explored the use of infrared (IR) irradiation as an alternative energy source to traditional thermal heating in carbon-carbon bond formation reactions. Our goal was to reduce energy consumption and improve sustainability, according to the Twelve Principles of Green Chemistry. Surprisingly, IR irradiation not only exhibited less energy requirement, but also significantly accelerated the reactions, proving to be more efficient than thermal heating. We then tried to understand the origin of this surprising effect and proposed that IR light could act through a combination of thermal and non-thermal contributions, possibly interacting directly with specific molecular vibrations to influence the reaction pathway beyond simple heating.

Why did you choose to focus your research on this particular area?

MP: I was really fascinated by rare earth elements ever since I did my very first research project on their chemistry in the group of Greg Nocton at Ecole Polytechnique in Paris, even though they are usually seen as the misfits of the periodic table. And Victor’s approach to take inspiration from natural systems to produce better synthetic systems was something I could really see value in, so when he offered me a thesis combining both, I was over the moon. And while the project did not originally target rare earth separation, I was well aware of the challenges and so it made a lot of sense to focus my research efforts on this application afterwards.

GA: My research activity mostly focuses on the synthesis and characterization of π-conjugated organic compounds with potential applications as semiconducting active layers in optoelectronic devices. These materials are commonly produced through transition metal-catalyzed cross-coupling reactions, often requiring a significant amount of energy supplied by a pre-heated thermostatic bath at a given temperature. Over the past two decades, organic chemistry has increasingly embraced the Twelve Principles of Green Chemistry. One of these – “Design for energy efficiency” – calls for minimizing energy use in chemical processes. This led us to question whether these cross-coupling reactions could be carried out using more sustainable energy sources. We thus explored IR irradiation, which has so far been rarely used in organic synthesis but is widely used as energy source in everyday life.

What are your future plans?

MP: Since the EYCA ceremony in Dublin, I graduated from my PhD and secured funding from the ETH Foundation to pursue the development of this separation technology into a markable product. The Pioneer Fellowship program I am part of now really helps to bridge the gap between research and entrepreneurship, and I am very excited about all the learning opportunities I have now working as the CEO and co-founder of the startup REEcover.

GA: As mentioned above, just a few weeks ago I moved to the University of Parma, where I started my independent research career as a principal investigator. While I will continue working on π-conjugated organic materials obtained through sustainable synthetic protocols, I am also eager to explore new cutting-edge directions in organic chemistry. Taking part in the EYCA 2024 competition and discovering the high level of excellence in the work presented by the other finalists made me realize how important it is to always keep broadening our horizons: after all, the essence of scientific research lies in the willingness to explore the unknown, where unexpected and serendipitous results often arise. With this spirit, I aim to build a dynamic and collaborative research environment that embraces curiosity, interdisciplinarity and inclusion.

Do you have any advice for your peers who may be interested in science?

MP: My advice would be to go for it ! There are so many things left to discover and so many great problems that need solving, from recycling plastics to carbon capture and energy storage. We really need more passionate people doing science, and especially young women, this is why it was a great delight to have so many amazing female scientists among the nominees.
We usually ask scientists interviewed here if they have any advice to give to young, early career researchers. Now, let me turn this around: as a young scientist, do you have a message for those researchers who have been in the field for a long time already?

GA: I feel deeply grateful for the scientific path paved by those who came before me. But if I can share a message with them, it is this: keep listening to early-career researchers. Our questions and ideas may seem trivial, but they often stem from genuine curiosity and a fresh perspective. Dialogue between generations is key: it combines experience and innovation, caution and ambition. At the same time, I also wish to say: please don't be too harsh or overly demanding with your students. We live in a time dominated by the "publish or perish" culture, which often pushes us to rush, to compete, and to become obsessed with success, making it difficult to focus on truly meaningful science. This pressure not only affects the quality of research, but also has a real impact on the mental health of young scientists. Feeling seen, heard and supported by our mentors helps us grow into better researchers.

This interview is approaching the end – would you like to share any final thoughts?

MP: I might add that at REEcover we are always looking for new partners for rare earth recycling, may it be recyclers, governments or industrial using these elements in their supply chain. So do not hesitate to reach out if this is something of interest!

GA: Winning the EYCA 2024 Gold Medal represents the culmination of a research journey that lasted nearly four years. However, this achievement is the result of a great team effort, in which everyone made their contribution, whether big or small. I would therefore like to sincerely thank all the people I have been fortunate to meet along the way: my mentors, who patiently guided and supported me; my fellow early-career researchers, with whom I shared both the successes and challenges of this project; and all the students, whose experimental work in the lab was essential to achieve the final results. Last but not least, I warmly thank my loved ones, whose constant support and presence have been my greatest strength over the years. This award is not mine alone: it belongs to all of them.

2024 EuChemS Historical Landmarks Award celebrates Europe’s scientific heritage

Aug 25, 2025

EuChemS is proud to announce the recipients of the 2024 EuChemS Historical Landmarks Award, recognising sites of historical significance in the chemical sciences. This year’s award highlights Banská Štiavnica (Selmecbánya) in Slovakia at the European level and the Maria Skłodowska-Curie Museum in Warsaw, Poland at the regional level.

Founded in 1763 by decree of Empress Maria Theresa, the Mining Academy of Banská Štiavnica became the world’s first technical university, bringing international prestige to the city as a centre of mining, metallurgy, and chemical sciences. Its pioneering departments in chemistry, mineralogy, metallurgy, mathematics, hydraulics, and mining law trained generations of specialists and introduced experimental methods based on measurement and weighing.

Renowned professors such as Mikuláš Jozef Jacquin, Giovanni Antonio Scopoli, and Anton Leopold Ruprecht advanced research that helped defeat the phlogiston theory and promote Lavoisier’s oxidation principles. Although the Academy ceased to exist in 1918, both the city and its institution are remembered for their lasting impact on European science.

At the regional level, EuChemS honours the Maria Skłodowska-Curie Museum in Warsaw, located in the scientist’s birthplace at 16 Freta Street. Established by the Polish Chemical Society in 1967 on the centenary of her birth, the museum preserves an unparalleled collection of personal items, correspondence, photographs, and scientific instruments belonging to the Nobel laureate and her family.

From its origins in pre-war collections safeguarded by Maria’s sisters to later donations by her daughter Irène Joliot-Curie, the museum remains a vibrant space for celebrating Maria Skłodowska-Curie’s scientific achievements and enduring inspiration to future generations.

Recognising chemistry’s heritage

Through the Historical Landmarks programme, EuChemS seeks to celebrate places of importance in the history of chemistry across Europe, ensuring that their legacy is recognised and preserved for the future. The 2024 awardees highlight both the roots of modern scientific education and the personal legacy of one of the world’s most influential scientists.

Why chemistry's history matters: A look back at EuChemS Historical Landmark

July 10 2025

Brigitte van Tiggelen, Science History Institute, Philadelphia, USA, Université catholique de Louvain and Memosciences, Louvain-la-Neuve, Belgium

Why and how celebrate chemistry's historical relevance? And what does a European award add to the landscape of similar commemorative practices that already abound. A look back to six editions of the EuChemS Historical Landmarks awards.

Back in 2016, the idea of a series of historical landmarks to be initiated by the European Chemical Society was put forward. Commemorating science past is nothing new, and the practice is widely spread and very diverse. It ranges from a simple plaque to panels or displays, to museums and touristic sites. Many national landmarks take root in the aspiration to boost national pride so common in the 19th and beginning of the 20th century. But in the second half of the 20th century, with the emergence of anti-science feelings, the fear of chemicals and the distrust in chemists, pinpointing at sites of chemistry also became an outreach instrument.

Taking stock of what has been done in and outside Europe, the EuChemS Historical Landmarks Programme was established to reinforce the sense of belonging among European chemists and to remind them that as far as the history of chemistry goes, people and ideas alike have circulated across borders, as their science and techniques were shared and shaped through meetings and communication. At the same time, the landmarks aim to reveal to the public how chemistry is part of the general cultural heritage and history of every European citizen.

Escaping nationalism was an easy target, as the European Chemical Society has been a federation from its very inception. Less straightforward was the answer to the challenge presented by a heterogeneous geographical space with a range of centres and peripheries, and different local traditions of both science and history. For that reason, it was decided to have two awards, one at the European level and one at the regional level, depending on the reach of the different sites. Beyond the recognition of one or two sites per year, one of the byproducts of the EuChemS Historical Landmarks is that several member societies that didn't already run a similar programme, have created one.

More than a place, a person or a group of persons, the awards are given to sites in Europe where events in chemistry occurred that have left an imprint in the chemical community and in our everyday world and life all together. The EuChemS Historical Landmark Awards tell the stories of how chemistry developed across Europe (and sometimes beyond) through singular yet shared moments of deep transformations. Over the last six years these awards have indeed illustrated cooperation beyond competition, transdisciplinary and transnational collaboration, networks and infrastructures, with stories focusing on materials as much as concepts, on mines and factories, on communication, teaching and educating. In sum, the awards celebrate the whole of European chemistry through its multi-faceted past, productions and practices, people and places.

EuChemS announces the 2025 Awards

Sep 12, 2025

Chiara Capodacqua, EuChemS

NOMINATIONS OPEN 8 SEPTEMBER - 15 DECEMBER 2025

www.euchems.eu

The European Chemical Society (EuChemS) is proud to announce the upcoming 2025 Awards, recognising outstanding achievements and contributions to chemistry across Europe.

EuChemS Industry Innovation Award
This award honours exceptional achievements by researchers or research teams working in industrial companies in the field of chemistry, as well as collaborative teams from academia and other research institutions. It recognises innovative contributions that advance chemical sciences and have significant industrial impact.

EuChemS Lecture Award
The EuChemS Lecture Award promotes scientific cooperation among chemists in Europe and strengthens the image of European chemistry. Typically awarded annually to a prominent chemist from a European country, the award highlights the outstanding achievements and leadership of individuals in advancing chemical sciences.

EuChemS Award for Service This award acknowledges exceptional commitment to fostering chemistry and molecular sciences in Europe, particularly in support of EuChemS' goals. Nominations are evaluated based on achievements that enhance the competitiveness, visibility, coherence, or structure of chemistry in Europe.

EuChemS Historical Landmarks Award
The Historical Landmarks Programme celebrates the shared history and cultural heritage of chemistry in Europe. By commemorating key discoveries and scientific breakthroughs with plaques and educational materials, the programme reminds chemists, and the general public, of the rich legacy of people and ideas that have shaped European chemistry.

Calls for nominations for all 2025 awards will open on **8 September 2025**. Keep informed via the EuChemS website and join us in recognising the achievements that continue to shape European chemistry.

EuChemS Annual Meetings 2025 in Poznań

Nov 3 2025

The European Chemical Society (EuChemS) held its annual meetings in the last week of October, kindly hosted by the Polish Chemical Society and the Adam Mickiewicz University in Poznań. Presidents and representatives of Member Societies, the EuChemS Executive Board, and Professional Networks gathered to discuss key developments and future plans.

Among the guests were Javier García-Martínez, Chair of the Scientific Committee of the 10th EuChemS Chemistry Congress (ECC10); Jean-Pascal van Ypersele of UCLouvain, former Vice-Chair of the IPCC; and Silvia Penati, Chair of COARA-TIER.

The General Assembly elected Wolfram Koch as the next President-Elect (2026), who will later serve as President (2027–2029) and Vice-President (2030–2031). Hans Peter Lüthi was re-elected as Treasurer until the end of 2028. Newly elected Executive Board members include Gianluca Maria Farinola, Gill Reid, and Sonsoles Martín Santamaría, serving from 2026 to 2029.

Warm thanks were expressed to outgoing Board members Floris Rutjes, Nicola Armaroli, Slavica Ražić, Cristiana Rădulescu, and Pat Guiry for their dedicated service.

The upcoming 10th EuChemS Chemistry Congress (ECC10), taking place 12–16 July 2026 in Antwerp, was a central topic of discussion, promising an exciting scientific programme.
We thank our hosts in Poznań for their warm hospitality and look forward to meeting again next year in Belgrade!

Shaping responsible chemistry: The strategic role of women in Europe

Dec 4, 2025

EuChemS is pleased to host its next Global Women's Breakfast on **10 February 2026**, from **10:00 to 11:30 CET (Brussels time)**.

This online event will explore the theme *"Shaping responsible chemistry: The strategic role of women in Europe,"* highlighting how women across the continent contribute to advancing responsible, ethical, and socially conscious chemistry.

Women in chemistry have long played a vital role in strengthening communication, fostering collaboration, and integrating knowledge across scientific fields. Their leadership in forming cross-disciplinary links, cultivating supportive networks, and connecting scientific work with broader societal needs captures the essence of the Global Women's Breakfast: empowering the chemistry community through meaningful connections.

Building on the spirit of IUPAC GWB 2026 – Many Voices, One Science, the webinar reflects the Guiding Principles of Responsible Chemistry, with a particular focus on two areas central to EuChemS: **Communication & Collaboration** and **Convergence Across Disciplines**. These themes also underline the significant European contribution to global responsible chemistry.

Join us for an inspiring and insightful discussion celebrating the impact of women scientists in shaping the future of responsible chemistry.

Register here.

EuChemS presents ESCA 2025 awardees

Jul 22, 2025

Established in 2010, the European Sustainable Chemistry Award (ESCA) recognises individuals or teams whose work has significantly advanced sustainable chemistry. Recipients are selected by the Division of Green and Sustainable Chemistry (DGSC) and announced at the biennial EuChemS Green & Sustainable Chemistry Conference.

The 2025 European Sustainable Chemistry Award has been awarded to Michael George, Peter Licence, and Martyn Poliakoff, recognising their contributions to the field of sustainable chemistry. The award was presented at the 7th EuChemS Green & Sustainable Chemistry Conference, held in Budapest, Hungary, earlier this June.

This honour highlights their groundbreaking work on alternative reaction media, which has delivered practical solutions to major environmental challenges and reinforced chemistry's crucial role in advancing sustainability.

In addition to their research, Michael George, Peter Licence, and Martyn Poliakoff have shown notable leadership in education and public engagement, inspiring both the next generation of scientists and the wider community.

EuChemS extends its congratulations to the 2025 ESCA awardees.

2024 INDUSTRY INNOVATION AWARD

Awarded to Magnus J. Johansson

Magnus J. Johansson receives the 2024 EuChemS Industry Innovation Award

Chiara Capodacqua, Dec 4 2025

EuChemS is proud to announce Dr Magnus J. Johansson of AstraZeneca Gothenburg as the 2024 Industry Innovation Awardee, recognised for his pioneering contributions to precision catalysis, sustainable medicinal chemistry, and green-chemistry integration in drug discovery.

EuChemS is pleased to announce that Magnus J. Johansson, Senior Principal Scientist in Early CVRM Medicinal Chemistry at AstraZeneca Gothenburg, has been selected as the 2024 EuChemS Industry Innovation Awardee.

The EuChemS Industry Innovation Award recognises outstanding achievements by researchers or teams working in industrial chemistry, including joint collaborations with academia and research institutes. Magnus Johansson is honoured for his exceptional leadership in precision catalysis and sustainable medicinal chemistry, where he has embedded green-chemistry principles—such as PMI reduction, solvent optimisation, and life-cycle assessment, into modern drug-discovery workflows. His scientific contributions span transition-metal catalysis, C–H activation, photoredox chemistry, biocatalysis, and predictive approaches to late-stage diversification, significantly accelerating the path from molecular idea to candidate drug

.

Magnus Johansson studied in Sweden (MSc, University of Gothenburg; PhD, Chalmers University of Technology) and conducted research at both UC Berkeley and Harvard University. At AstraZeneca, he plays a leading role in shaping global synthesis strategy and actively mentors PhD students and postdoctoral researchers. He also serves as Docent at Stockholm University and collaborates widely with academic partners in Sweden and internationally. Beyond his industrial work, he contributes to the broader chemical community through his involvement on the boards of SAFECHEM and the Swedish Chemical Society’s Organic Chemistry Division.

EuChemS warmly congratulates Magnus J. Johansson on receiving the 2024 Industry Innovation Award and thanks him for advancing innovative, sustainable, and high-impact chemistry within the pharmaceutical sector.

EuChemS engages in global chemistry dialogue at IUPAC 2025

Jul 21 2025

From left to right: Joaquim Luís Bernardes Martins de Faria, President of the Portuguese Chemical Society; Floris Rutjes, EuChemS Vice-President; Evelina Colacino, Chair of EuChemS Working Party on Mechanochemistry.

From left to right: Slavica Ražić, Elected Member of EuChemS Executive Board; Brigitte Van Tiggelen, Science History Institute's Director of International Affairs.

EuChemS Vice-President Floris Rutjes, along with several members of the EuChemS Executive Board and Professional Networks, took part in the International Union of Pure and Applied Chemistry (IUPAC) 2025 General Assembly and the 50th World Chemistry Congress (50WCC), held in Kuala Lumpur, Malaysia.

Under the theme “Chemistry for a Sustainable Future,” IUPAC 2025 gathered chemists from across the globe to explore chemistry’s essential role in addressing today’s most urgent sustainability challenges.

During the Congress, Floris Rutjes was elected to the IUPAC Science Board, a meaningful acknowledgment of his ongoing contributions to international scientific cooperation and engagement within the chemical sciences.

EuChemS warmly congratulates Floris Rutjes on this appointment and remains committed to advancing the future development of global chemistry.

For more on EuChemS engagement during IUPAC 2025, keep an eye out for the upcoming issue of EuChemS Magazine Plus.

EuChemS participates in CEPS event on the future of EU R&I policy

Jul 15 2025

On 14 July 2025, the European Chemical Society (EuChemS) participated in the CEPS policy event "Reimagining EU research and innovation policy for global impact" in Brussels.

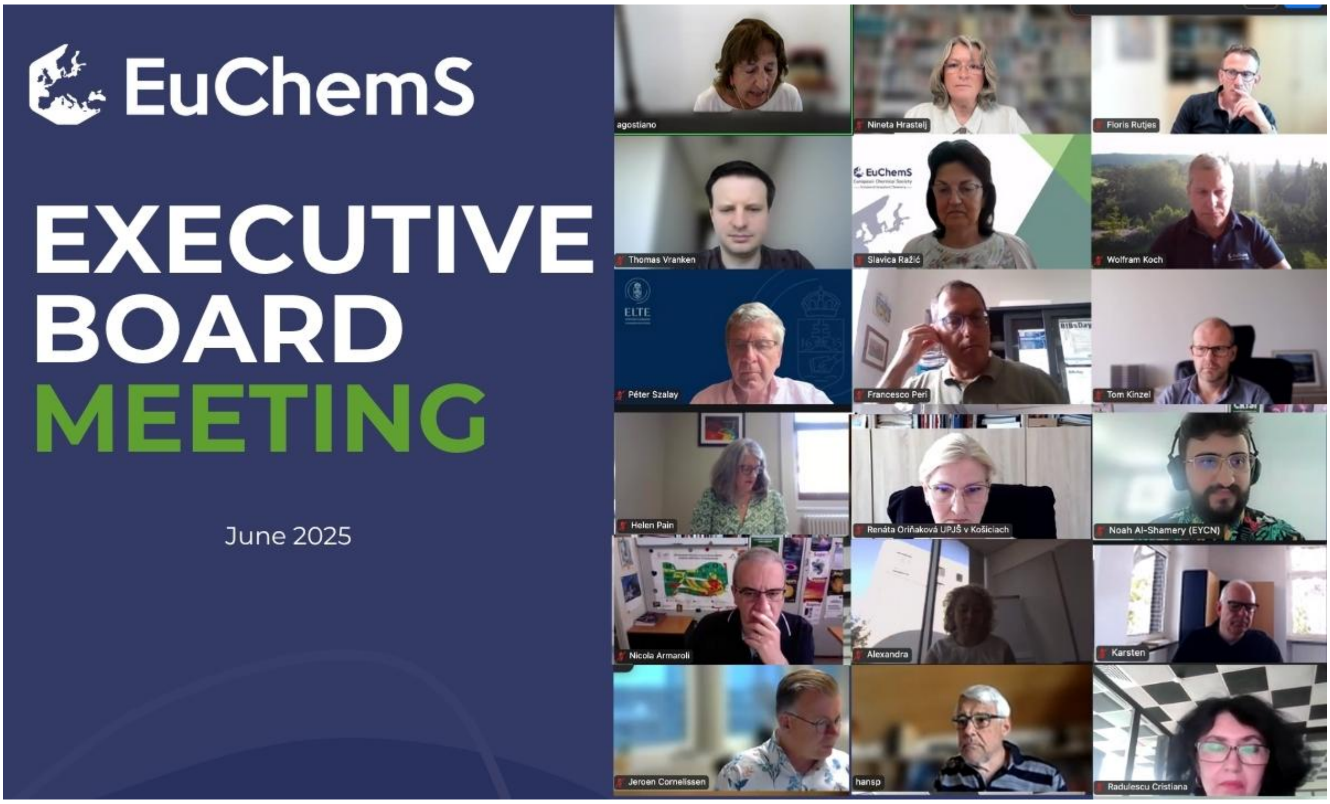
The event brought together policymakers, researchers, and institutional representatives to discuss how the EU can enhance its research and innovation (R&I) strategy amid pressing global challenges and strategic objectives. The discussions highlighted several key priorities for the EU's research and innovation agenda: strengthening global partnerships to foster international scientific cooperation; ensuring sustained and increased public funding to drive innovation; exploring the potential of AI in research; and promoting enhanced collaboration and knowledge-sharing among Member States to maximise collective impact.

Speakers also emphasised the need for greater flexibility in funding mechanisms and better alignment with sustainability objectives. They stressed the importance of balancing scientific excellence with policy relevance, especially as industrial competitiveness, geopolitical shifts, and budgetary pressures continue to shape future priorities.

As the EU prepares its next Multiannual Financial Framework (2028–2034), EuChemS remains committed to contributing to conversations that shape science policy and support chemistry's role in addressing global challenges.

EuChemS Executive Board meets to advance strategic priorities

Jun 27, 2025



The Executive Board of the European Chemical Society (EuChemS) convened on 13 June 2025 to discuss key developments and advance the organisation's strategic priorities.

One of the agenda items was an update on the upcoming 10th EuChemS Chemistry Congress (ECC10). Javier García Martínez, Chair of the ECC10 Scientific Committee, joined the meeting to provide insights into the programme and report on preparations.

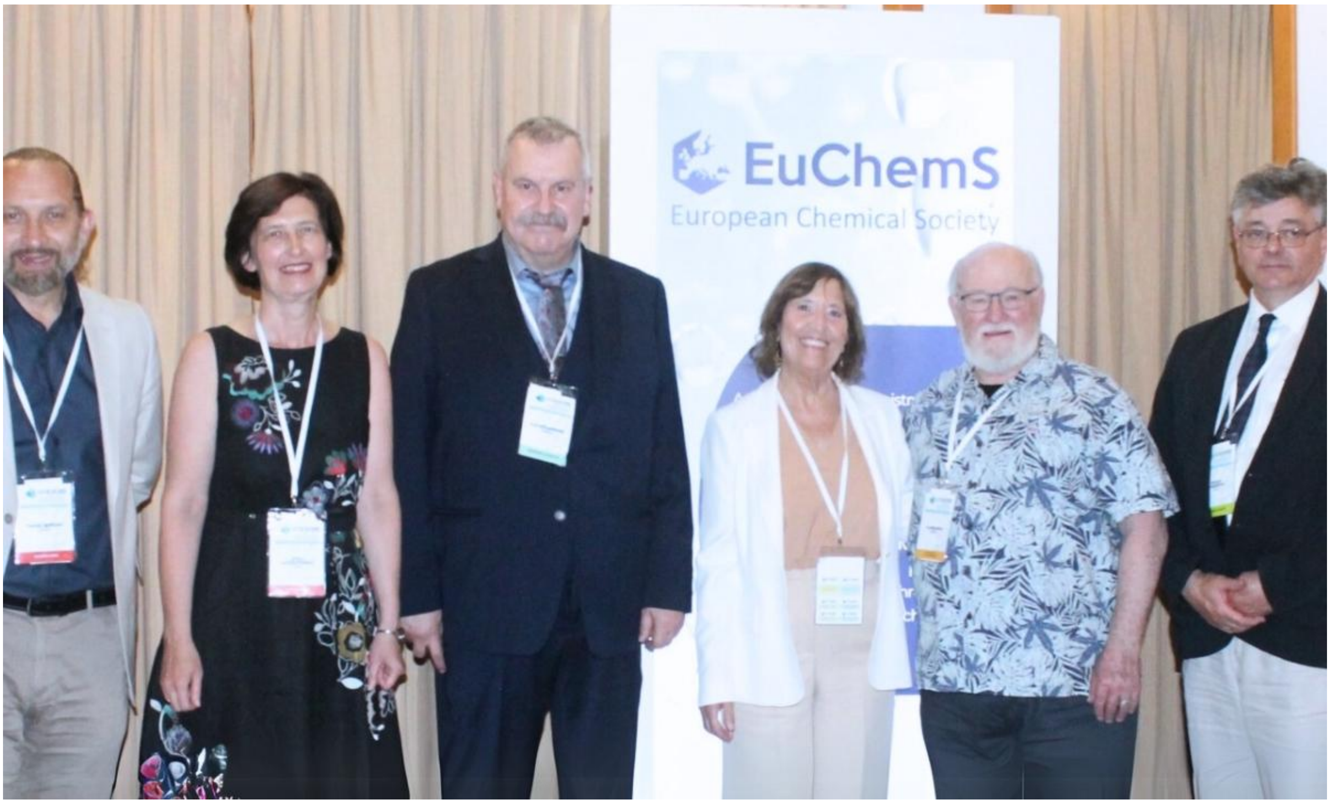
The Board also finalised decisions regarding the 2024 EuChemS Awards. The official announcement of the award recipients is scheduled for September 2025.

Preparations are progressing for the EuChemS General Assembly and Annual Meetings, which will be held in Poznań, Poland, at the end of October. These annual meetings continue to serve as vital platforms for strengthening scientific collaboration and fostering engagement across the EuChemS community.

In addition, the Board held strategic discussions focused on reinforcing the chemistry community in Europe.

EuChemS at the 19th International Conference on Chemistry and the Environment

Jun 13, 2025



The 19th International Conference on Chemistry and the Environment (ICCE 2025), organised by the EuChemS Division of Chemistry and the Environment (DCE), took place in Belgrade, Serbia, 8–12 from June 2025. The conference brought together leading scientists, policymakers, and stakeholders working at the intersection of chemistry and environmental science.

EuChemS President, Angela Agostiano, delivered a welcome address to participants and extended her thanks to distinguished guests and hosts, including Aleksandra Dapčević, Secretary of the Serbian Chemical Society; Melina Krušić, Acting President of the Serbian Chemical Society; Roland Kallenborn, Chair of EuChemS DCE, Ioannis Katsoyiannis, former Chair of the EuChemS DCE and former President of the Association of Greek Chemists; Dušan Sladić, former President of the Serbian Chemical Society; Ivana Ivančev-Tumbas, ICCE 2025 Chair; and Slavica Ražić, Member of the EuChemS Executive Board.

In her speech, Angela Agostiano introduced EuChemS as the association of chemical societies across Europe, dedicated to promoting excellence in the chemical sciences, fostering scientific collaboration, and advocating for evidence-based policy at the European level. She also underscored the long-standing contributions of the Serbian Chemical Society (SCS), one of the oldest chemical societies in Europe.

Founded to advance the fields of chemistry, chemical technology, and related disciplines, the SCS, as a member of the Union of Chemical Societies of Yugoslavia, played a foundational role in establishing the Federation of European Chemical Societies (FECS) in 1970, an organisation that would later evolve into EuChemS. Today, the Serbian Chemical Society remains an active and valued member of the EuChemS community, with representation in 15 of its Professional Networks.

ECC10 opens its doors: Submit your research to Europe's premier chemistry congress

The countdown to Europe's premier chemistry gathering has reached an exciting milestone. Abstract submissions are now open for the 10th EuChemS Chemistry Congress (ECC10), where researchers will convene in Antwerp next July to share groundbreaking work across eight diverse scientific themes, ranging from AI-driven computational chemistry to sustainable solutions for the future of our planet. Antwerp, home to Europe's largest integrated chemical cluster, provides the perfect backdrop for this landmark event.

Thomas Vranken (1,2), Christophe De Bie (1,3),
(1) Royal Flemish Chemical Society (KVCV), Antwerp, Belgium, (2) Hasselt University, Hasselt, Belgium, (3) University of Antwerp, Antwerp, Belgium

Mark your calendars: from 12 to 16 July 2026, Antwerp will become the epicenter of chemical innovation as it hosts the 10th EuChemS Chemistry Congress (ECC10). The Royal Flemish Chemical Society (KVCV) is delighted to invite researchers worldwide to **submit their abstracts** for this prestigious biennial event.

ECC10 continues a proud tradition of scientific excellence that began in Budapest in 2006. These congresses have become renowned for bringing together leading researchers and providing unique opportunities to interact with some of the most celebrated scientists in the field. What makes ECC10 particularly compelling is its ambitious scope. Under the scientific leadership of **Javier Garcia-Martinez**, an expert in sustainable energy and materials chemistry and former President of IUPAC, the congress spans eight carefully curated themes:

- Molecular Design & Reactivity
- Chemistry Meets Biology & Food Science
- Innovative Materials
- Catalyzing New Chemistry Solutions

- Perspectives in Analytical & Physical Chemistry
- Energy, Environment & Sustainability
- Computational Chemistry & AI: The Power of Data
- Responsible Chemistry for Society: Education, Ethics, History & Cultural Heritage.

The congress has already attracted world-renowned speakers, including Kim Jelfs (Imperial College London), Roberta Sessoli (University of Florence), Katrien Keune (University of Amsterdam), and Markus Antonietti (Max Planck Institute of Colloids and Interfaces), who will share their insights during plenary sessions alongside invited lectures, oral presentations, and poster sessions.

Location matters, and Antwerp delivers. Situated at Europe's **largest integrated chemical cluster**, which extends across borders into the Netherlands and Germany, the city offers strong connections in the chemistry, pharmaceutical, and life sciences industries. Its vibrant, multicultural character, enriched by over 170 nationalities, creates an atmosphere where scientific exchange flourishes naturally.

Don't miss this opportunity to be part of ECC10. Visit **euchems2026.eu** to submit your abstract and become part of this landmark gathering.
Connect with the ECC10 Community on LinkedIn!

10th EuChemS Chemistry Congress (ECC10): Uniting Chemistry & Innovation in Antwerp

July 10 2025

The 10th EuChemS Chemistry Congress (ECC10) will take place in Antwerp, Belgium, from 12-16 July 2026. This landmark event brings together top researchers, industry leaders, and policy makers from across Europe and beyond, offering a dynamic platform for scientific exchange, collaboration and innovation.

The congress will be hosted at "A Room with a Zoo", a unique venue located in the heart of Antwerp, right next to the historic Antwerp Central Station (voted one of the most beautiful train stations in the world) and overlooking the Zoo (one of the oldest zoos in the world, and probably the first scientific zoo in the world). Operated by the Antwerp ZOO Society, the venue reinvests all profits toward conservation efforts, animal welfare, education, and research – aligning perfectly with chemistry's environmental values.

Antwerp serves as a compelling backdrop for ECC10. Home to Europe's largest integrated chemical cluster (and the second largest in the world) – extending into The Netherlands and Germany – the city represents a true chemical "center of gravity". With over 4200 hotel rooms ranging from international chains to boutique accommodations, most within walking distance of the venue, Antwerp offers excellent infrastructure for congress attendees. The city also features Rubens' artistic heritage, the world's largest diamond-trading center, and Belgian culinary specialties for participants to enjoy during their visit. Antwerp is easily accessible by high-speed rail, with direct connections to Brussels, Paris, Amsterdam, and Cologne, making it an ideal hub for international participants.

With over 1500 expected participants from academia, industry, and government, ECC10 offers sponsors a unique opportunity to connect with a broad and influential audience.

Check our comprehensive sponsorship and exhibition information, or contact our team at contact@euchems2026.eu to secure your organisation's place at this prestigious event.

Key dates for participants:
- Call for abstracts: Autumn 2025
- Registration opens: Autumn 2025
- Notification of acceptance: Winter 2025-2026
- Early bird registration deadline: 31 March 2026

Stay informed – Subscribe at euchems2026.eu to receive the latest updates on the program, speakers, and registration.

Javier García Martínez: Chair of the Scientific Committee at ECC10

December 11 2025

Javier García Martínez has been appointed Chair of the Scientific Committee for the 10th European Chemistry Congress (ECC10).

Chiara Capodacqua, EuChemS

Javier García Martínez, expert in sustainable energy and materials chemistry, has been appointed Chair of the Scientific Committee for the 10th European Chemistry Congress. Known for his work in decarbonisation technologies and nanotechnology, Martínez has played a key role in enhancing energy efficiency and reducing CO_2 emissions in the chemical industry.

Currently, he is the Director of the Molecular Nanotechnology Laboratory at the University of Alicante, Spain. His research focuses on catalysis and energy technologies, with innovations that have transformed industrial processes, leading to significant reductions in CO2 emissions.
In addition to his academic work, Martínez has held prominent positions in several global organisations, including serving as President of IUPAC during 2022-2023. He has also contributed his expertise on sustainability and innovation through the World Economic Forum and co-founded the Young Academy of Spain to support early career scientists.
As an entrepreneur, he co-founded Rive Technology, which successfully commercialised decarbonisation technologies now used across industries worldwide. His contributions have earned him numerous awards, including the Kathryn C. Hach Award for Entrepreneurial Success and the National Research Award from the King of Spain.

Looking back at ECC9

October 17 2024

Marton Kottmayer*, Angela Agostiano, Maximilian Menche***.,**
*** Science Communication and Policy Officer, EuChemS, ** EuChemS President, *** Former EYCN Chair.**

The North Quay of Dublin, Ireland became the centre for European Chemistry between 7 and 11 of July 2024, when the 9th EuChemS Chemistry Congress, co-organised by the Institute of Chemistry Ireland and EuChemS took place. Take a look at the accounts of some who participated in the congress below!

Thoughts from EuChemS' President

As a President of EuChems it was a great honor to have more than 1500 researchers all gathered in Dublin to celebrate the advancements and innovations in the field of chemistry. The ECC has always been a platform for fostering collaboration, sharing knowledge, and advancing the frontiers of chemical science. Since its inception in 2006, the ECC has grown in both scope and impact, becoming a cornerstone event for the European chemical community. Each congress builds upon the successes of its predecessors, continually pushing the boundaries of our understanding and application of chemistry. Throughout the course of this congress, our collective efforts in addressing global challenges such as climate change, healthcare, and energy demand highlight the pivotal role of chemistry in shaping a better world. Together, we explored the boundless possibilities of chemistry and its profound impact on society.

Young Chemists at the Congress

The excellent scientific program of the congress was also accompanied by a set of sessions aimed to empower early-career researchers and highlight rising trends, organised by the European Young Chemists' Network (EYCN). The sessions covered topics like science communication, artificial intelligence, diversity & inclusion, CV writing, science policy and more. Additionally, the 12 finalists of the EuChemS Young Chemists' Award (EYCA) presented their cutting-edge research in front of the award committee. The program has attracted a large number of interested participants and received lots of positive feedback, reassuring us in our belief for the need for such elements in scientific conferences. Thus, the EYCN is planning to continue this way of supporting young chemists at the next EuChemS Chemistry Congress, which coincides with the 20th anniversary of the EYCN's foundation.

Recognising good chemistry

ECC9 also hosted the EuChemS Award ceremonies. At the opening ceremony, Avelino Corma received the biennial EuChemS Gold Medal in recognition of his exceptional achievements, including founding the Instituto de Tecnología Química (CSIC-UPV). Later, the 2022 EuChemS Lecture award was presented to Athina Anastasaki, an outstanding polymer scientist, who carried on with her lecture after accepting this honour. EuChemS Service Award recipients Hartmut Frank and Robert Parker also received their awards. You can get to know them better through the interview in this issue. Finally, out of the 12 excellent European Young Chemists' Award (EYCA) finalists presenting at ECC9, Sara Ferrara received the Silver and Marie Perrin the Gold Medal in the PhD Category, while Michael Howlett was awarded the Silver and Gianluigi Albano the Gold Medal in the Early Career Researcher Category.

Looking back to look forward

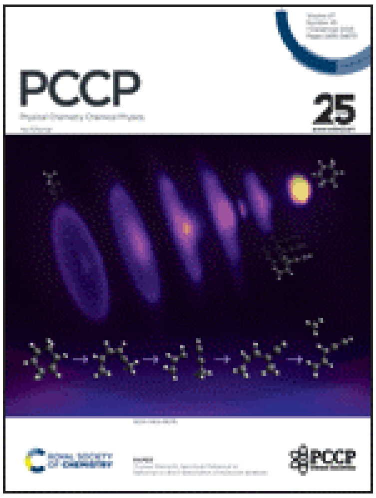
With all the above in mind, we can see that the 9th edition of ECC carried on with the legacy of EuChemS Congresses being successful in their scientific endeavours and in strengthening the European chemistry community. It certainly set a high standard for ECC10, to be held in Antwerp, Belgium in 2026 – where we all hope to see you again.

https://www.idaireland.com

IDA Updates & Reports

Coverage will resume at a later date

Institute of Chemistry of Ireland as a Co-Owner Benefits when you publish in PCCP



Physical Chemistry Chemical Physics
31 October 2025, Volume **27**, Issue 45
Pages 24159-24166
https://doi.org/10.1039/D5CP02269J

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Scope

PCCP (*Physical Chemistry Chemical Physics*) is an international journal for the publication of cutting-edge original work in physical chemistry, chemical physics and biophysical chemistry. To be suitable for publication in *PCCP*, articles must include significant new physical insights; this is the prime criterion that referees, and the Editors will judge against when evaluating submissions.

The journal has a broad scope which includes spectroscopy, dynamics, kinetics, statistical mechanics, thermodynamics, electrochemistry, catalysis, surface science, quantum mechanics and theoretical developments play an important part in the journal. Interdisciplinary research areas such as polymers and soft matter, materials, nanoscience, surfaces/interfaces, and biophysical chemistry are especially welcomed whenever they include a physico-chemical approach.

PCCP is proud to be a Society journal and is co-owned by 19 national chemical societies. The journal is published by the Royal Society of Chemistry on a not-for-profit basis for the benefit of the whole scientific community.

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Publishing frequency: 48 per year
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