UCC University College Cork, Ireland
Coláiste na hOllscoile Corcaigh

Department of Chemistry

68th Irish Universities Chemistry Research Colloquium

23rd & 24th June 2016

University College Cork

Book of Abstracts

Participating Institutions

Organizing Committee

Colm O'Dwyer (Chair)

Christine Dennehy

Trevor Carey

Stuart Collins

Claire Tobin

Órla Ní Dhubhghaill

Aisling Prendergast

Dave Otway

Eric Moore

Justin Holmes

Conference Website

https://www.ucc.ie/en/chemistry/chemistry-colloquium-2016/

68th Irish Universities Chemistry Research Colloquium

June 23rd & 24th, 2016.

UCC and the Chemistry Department would like to thank all our sponsors for their generous support.

General Information

The 68th Irish Universities Chemistry Research Colloquium will take place on Thursday 23rd and Friday 24th of June, 2016. Should you have any queries during the Colloquium, which are not answered below, please contact one of the Colloquium organisers at our information desk or call the departmental office on 021-4903764. The information desk will be manned in the foyer of the Boole Theatre, see map, during the coffee breaks. Refer to the colloquium website for further details and information.

Registration

Registration will take place in the Aula Maxima on Wednesday 22nd of June from **6.00-8.00 pm** and also in the Boole Theatre foyer on Thursday 23rd June at **8.45 am**. Each delegate will receive a welcome pack on registration. Speakers should present themselves to the Colloquium organisers at the registration desk.

Oral Presentation Sessions

The oral presentations will be held in parallel sessions in the Boole Lecture Theatres 3 and 4, see maps, beginning at **9.30 am** on Thursday. Please arrive at the beginning of each session so as not to disturb the speakers. The details and times of talks and flash presentations are outlined in the programme. All speakers of talks and flash presentations must upload their talks to the podium PC during the preceding coffee break/interval.

Poster Session

The poster session takes place on Thursday 23rd of June at **5.10 pm** until **6.10 pm** in the Kampus Kitchen Hall on the Basement Level of the Kane Building. All poster presenters should have posters already displayed and be available for discussion throughout the poster session.

Delegates presenting posters should mount their display on the poster boards in the Kampus Kitchen, see map, on the morning of Thursday 23rd of June from **8.45 am**. Posters (A0 in size, portrait orientation) should be displayed according to assigned numbers on the abstracts.

Coffee Breaks

There are coffee breaks at **11.25 am** and **3.30 pm** on Thursday, and **10.45 am** on Friday. The coffee breaks will take place in the foyer of the Boole Theatre Area.

Lunch

There are several cafes and restaurants on and around UCC campus where delegates may wish to have lunch. Cork city centre is approx. 15 min walk from UCC.

Colloquium Barbeque

The Colloquium barbeque will take place at the River Lee Hotel on the Thursday evening. The hotel is approx. a 10 minute walk from the main UCC gates. The welcome pack contains your barbeque ticket, which must be presented to gain access to this event. Delegates are asked to be in the Weir Bar at the River Lee Hotel by **8.00 pm**.

Banking and Parking

There are two ATMs on the main campus (see maps provided and linked on the colloquium website – one located outside the Main Student Restaurant, the other within the Student Centre). Limited parking is available on campus in both Visitors Car Parks. Accessible parking where required are detailed on the website.

Internet Facilities

Visitors coming from another college should be able to automatically access Eduroam Wi-Fi. In the event of a student of visitor not having Eduroam, access to the UCC Guest Wi-Fi is as follows:

Username: **chem23june16** Password: **v2dzNd9q**

Award Ceremony and Closing Address

The Closing Keynote Talk, award ceremony and closing address will be held in Boole Theatre 3 on Friday 24th of June at **11.15 am**. All delegates should attend and any presenters who are unavailable to attend should nominate a person to collect a prize in their absence.

Speaker Indemnification: The ideas and opinions expressed in the technical sessions and posters are those of the presenter. No endorsement by the chemistry Department, sponsors, or UCC can be claimed.

Photography and Recording is not Permitted in Technical or Poster Sessions

THURSDAY 23rd

8.45 am	Registration
	Boole 3
9.30 am	Welcome and Opening Remarks Prof. Justin D. Holmes *Head of Chemistry*
	Plenary Lecture
9.45am	Prof. John Sodeau *Every Breath You Take*

	Boole 3	**Boole 4**
	CHAIR: Dr Paul Evans	**CHAIR: Dr Orla Ni Dhubhghaill**
10.35am	Aramballi Jayanth, S. (TCD) *Self assembly studies of tripodal molecules towards new materials*	Gibson, Gregory (QUB) *The Electrochemical Generation of O_3 on a Ni/Sb-SnO_2 Electrode: A DFT Study*
11.00am	O'Shea, Kevin (UCC) *Synthesis & Evaluation of Novel Functionalized Indoles as Potential Inhibitors of Kinase*	Wilson, Eoin (UCC) *Investigation of the near-UV optical properties of secondary organic aerosols in an atmospheric chamber*
11.25am	Coffee Break	
	CHAIR: Dr Ger McGlacken	**CHAIR: Prof. Martyn Pemble**
11.55am	Reddy, Andrew (Maynooth) *Synthesis, Characterization and In Vitro Anti-parasitic Activity of a Novel Family of Glycosylated Metallodrugs*	Liu, Pai (UL) *Device Scale Assembly of Semiconductor Nanorods by Electrophoretic deposition*
12.20pm	Smith, Raymond (UCD) *Configuration-Based Orthogonal Activation of Thioglycosides*	Sarangapani, Chaitanya (DIT) *Non-thermal plasma: a novel chemical decontamination tool*
	Flash Talks 1	
	CHAIR: Dr Dara Fitzpatrick	**CHAIR: Dr Tony Keene**
12.45pm	Helen, Lisa (Tyndall/UCC) *The 'Smart' Needle – A Needle Integrated with an Impedance Sensor for Objective Nerve Localisation during Ultrasound Guided Peripheral Nerve Block*	Browne, Michelle (TCD) *Water Splitting at Transition Metal Oxide (TMO) Films in Alkaline Media - Cost vs. Activity*

	Ahmed, Muhib (Maynooth) *New Life for an Old Tuberculosis Drug*	Buk, Vuslat (Tyndall) *Novel miniaturized gold microelectrodes for electrochemical detection of hydrogen peroxide*
	Kitteringham, Eolann (RCSI) *Development of Bespoke Metal Complexes for Cellular Targeting*	Heffernan, Maria (UL) *Electroactive Bioresorbable Materials for Tissue Engineering Scaffolds*
	Gaynor, Brian (UCD) *In Silico Determination of Dioxygen Addition to a (Cp*)Ru(II) β-diketiminate Complex*	Newman, Gemma (ITT) *Design and Evaluation of New Biomaterials to Treat Fungal Infection*
1.05pm	Lunch	
	CHAIR: Dr Stuart Collins	**CHAIR: Prof. John Cassidy**
2.15pm	Ramos, Jessica (Maynooth) *Selective aliphatic/aromatic organogelation controlled by the side-chain protection of serine amphiphiles*	Ryan, Catherine (UCC/Tyndall) *An organic-inorganic composite designed for pH-driven optical detection by combination of chitosan and colloidal silica*
2.40pm	Antonik, Pawel (NUIG) *Lectin–Glycopolymer Interactions as a Route to Noncovalent PEGylation*	Ford, Rochelle (UCD) *Design and characterization of amperometric glutamate biosensors*
3.05pm	McKeon, Aoife (RCSI) *Pt Anticancer Compounds; Targeting HSP70-1*	Kyne, Michelle (NUIG) *Fluorescence Emission Properties of Triazine Fluorophores in Micelle and Protein Solutions: A Comparison*
3.30pm	Coffee Break	
	CHAIR: Dr Simon Lawrence	**CHAIR: Dr Eric Moore**
4.00pm	Conway-Kenny, Robert (TCD) *Synthetic Potential; Large Poly-Phenyl Ligands Derived from 1,10-Phenanthroline*	McCrellis, Corina (QUB) *Effect of the Presence of MEA on CO2 Capture Ability of Superbasic Ionic Liquids*
4.25pm	Zhang, Shi Yuan (UL) *A Chiral Crystalline Sponge*	Cheung, Shane (RCSI) *Real-time Imaging of Lysosomal Disruption with a pH Responsive NIR Fluorophore*

	Flash Talks 2	
	CHAIR: Dr Micheal Scanlon	**CHAIR: Dr Colm O'Dwyer**
4.50pm	Mulahmetovic, Ensar (DIT) *Synthesis of Novel Magnetic Catalysts*	Pettenuzo, Andrea (NUIG) *Recent Developments of Gold(III) Dithiocarbamato Glycoconjugates for the Targeted Metal-Based Anticancer Chemotherapy*
	Molphy, Zara (DCU) *DNA Oxidation Profiles of Copper Phenanthrene Chemical Nucleases*	O'Connell, John (UCC) *Monolayer doping of Si and $InGa_{0.53}As_{0.47}$ substrates and devices for future CMOS applications*
	Jinju, James (UCD) *Catalytic asymmetric synthesis of sterically hindered a-allyl-a-aryl lactones*	Creedon, Niamh (Tyndall) *Nanowire-based, Label-free Electrochemical Detection of Bovine Respiratory Disease Pathogens in Serum*
	Kampus Kitchen	
5.10pm	**Poster Session**	
6.10pm	Finish Day 1	
	River Lee Hotel (Weir Bar)	
8.00pm	**BBQ**	

FRIDAY 24th

	Boole 3	**Boole 4**
	CHAIR: Dr Colm O'Dwyer	**CHAIR: Dr Nikolay Petkov**
9.55am	Slator, Creina (DCU) *[Cu(o-phthalate)(phenanthroline)] Exhibits Unique Superoxide-Mediated NCI-60 Chemotherapeutic Action through Genomic DNA Damage and Mitochondrial Dysfunction*	Bruen, Danielle (DCU) - *Applications of Fluorescent Biosensors for Non-Invasive Glucose Monitoring*
10.20am	Belhout, Samir (UCD) *Preparation and Characterisation of Supported Gold Nanoparticles with Tunable Loading and Various Applications*	McCarney, Eoin (TCD) *Synthesis of functional supramolecular architectures the development of healable luminescent metallogels from triazole- based heterocyclic ligands*
10.45am	Coffee Break	

Boole 3	
	Keynote Speaker
11.15am	Dr Dara Fitzpatrick *A Sound Approach to Analytical Chemistry*
12.00pm	Award Presentations
	Closing Remarks Prof. Anita Maguire *Vice President for Research & Innovation*

Thursday, June 23rd

Opening Session

BOOLE 3

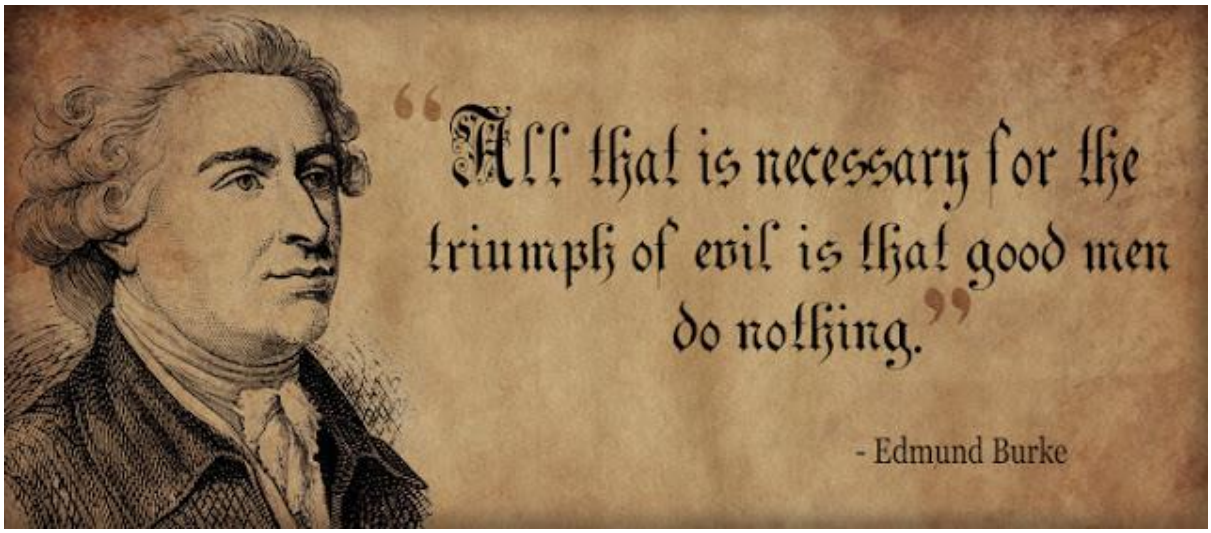
Welcoming Remarks &

Plenary Talk

9.30 – 10.35 am

Every breath you take

Sodeau, J.R.
Department of Chemistry and Environmental Research Institute, UCC



Abstract:

Why does our Air need care? The answer to this question will be discussed in the context of Health & Wellness and also Climate Change.

Air Quality is defined by the amounts and types of gases, vapours, aerosol droplets and solids that reside in our atmosphere. Their residence times and subsequent effects on our environment depend on "pollutant" sources (natural and anthropogenic) and sinks (chemical and physical). Their impacts can lead to wide ranging effects on us: cancer, cardiac arrest, asthma, headaches, flooding, drought, extreme weather events……the list goes on.

Unfortunately, our national and international responses to these problems depend on the actions of politicians who mainly have little understanding of either the fundamentals or the complexities associated with atmospheric chemistry, atmospheric physics, aerobiology, computational modelling and environmental engineering.

So it is up to us all as scientists, engineers and technologists to urgently inform the public about the consequences that air pollutants can have on us and planet Earth. It is time for us to do more.

Email: j.sodeau@ucc.ie

Session 1

BOOLE 3 & 4

Parallel Sessions

(Talks)

10.35 – 11.25 am

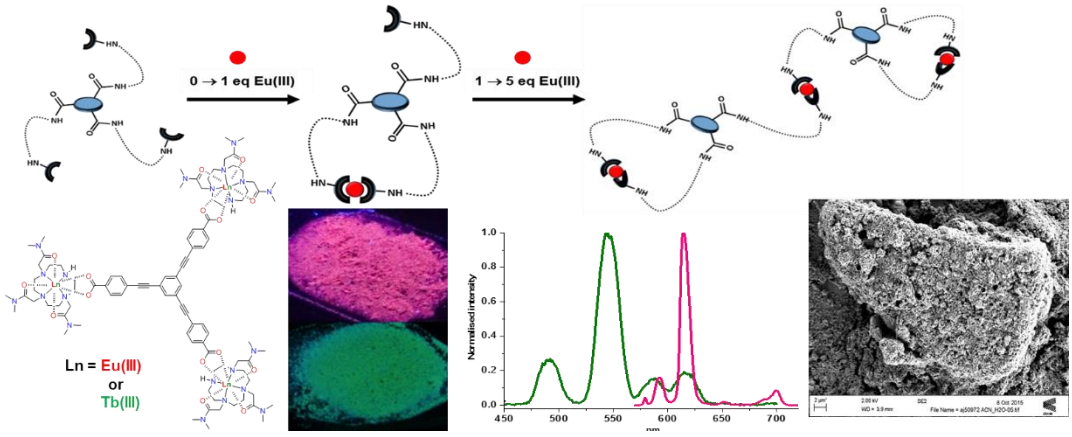
Self-Assembly Studies of Tripodal Ligands: Towards Co-Ordination Polymers and Luminescent Materials

Aramballi Jayanth, S.;[*a] Kotova, O.;[a] Caffrey, D.;[a] Boland, J.J.;[b] and Gunnlaugsson, T.[a]
[a] *School of Chemistry and TBSI, Trinity College, Dublin, Ireland*
[b] *School of Chemistry and Centre for Research on Adaptive Nanostructures and Nanodevices, Trinity College, Dublin, Ireland*

Abstract:

Self-assembly of organic molecules into well-defined organized structures has attracted considerable research interest towards the development of new materials and their applications in diverse fields such as molecular electronics, light-energy conversion, catalysis, soft materials and drug delivery systems.[1-4]

We have shown the formation of supramolecular coordination polymers based on terpyridine based tripodal C_3-symmetrical ligands (L) and europium ions (Eu(III)). The synthesis of the *ligands* was carried out in 5 steps with high yield. The complexation process between Eu(III) and ligands in both lower ($c = 5 \times 10^{-6}$ M) and higher ($c = 1 \times 10^{-5}$ M) concentrations were observed through spectrophotometric titrations conducted in MeOH. The binding model of stepwise addition of metal was obtained by fitting the titration changes using nonlinear regression analysis program SPECFIT. Of these, the changes in the absorption spectra gave excellent fits and the binding constants obtained for the 1:1, 2:1, and 3:1 (M:L) species with $log\beta_{1:1} = 8.49 \pm 0.16$, $log\beta_{2:1} = 15.6 \pm 0.17$ and $log\beta_{3:1} = 20.6 \pm 0.19$ at $C_L=5\times10^{-6}$M. Similarly, the binding constants for 1:1 and 3:2 species were $log\beta_{1:1} = 6.31 \pm 0.39$, $log\beta_{3:2} = 26.0 \pm 0.39$ at $C_L=1\times10^{-5}$M.



References:

1 Aida, T.; Meijer, E, W.; and Stupp, S, I. *Science*., 2012 (335) 813.
2 Badjić, J, D.; Balzani, V.; Credi, A.; Silvi, S and Stoddart, J, F. *Science*., 2004, (303), 1845.
3 Bunzli, J.C.G.; and Piguet, C. *Chem. Soc. Rev.*, 2005, (34), 1048.
4 Kotova, O.; Daly, R.; dos Santos, C. M. G.; Boese, M.; Kruger, P. E.; Boland, J. J.; and Gunnlaugsson, T. *Angew. Chem. Int. Ed.*, 2012, (51), 7208.

Email: ajsa@tcd.ie.

The Electrochemical Generation of O_3 on a Ni/Sb-SnO_2 Electrode: A DFT Study

Gibson, G.*; Hu, P.; Hardacre, C.; Lin, W.F.
Queen's University Belfast

Abstract:

For the past few decades the production of Ozone (O_3) via a water splitting mechanism at room temperature has been reported as a genuine alternative to the more traditional method current used, a Cold Corona Reactor (CCD).[1,2] By careful choice of catalyst, O_3 efficiencies have far surpassed that of the CCD method.[3,4] To date, literature studies have determined that the catalyst that exhibits the highest current efficiency for O_3 formation is Ni/Sb-SnO_2. In this work, the formation of O_3 from H_2O has been investigated. Literature studies show many examples portraying high O_3 yields, but show little understanding into the mechanism, apart from postulating how the mechanism will proceed. Using Density Functional theory (DFT), we have taken this mechanism and studied each step individually to gain a better understanding of what is going on at the quantum level. Previous studies by our group on β-PbO_2 have shown that the final step in the reaction (the formation of O_3) occurs via an Eley-Rideal style interaction where surface O_2 desorbs and then attacks surface bridging O• to form O_3.[5] Using what we have learnt from this study, we expected the Ni/Sb-SnO_2 to proceed in a similar manner. This was not the case, as with the Ni/Sb-SnO_2 surface, a Mars-Van Krevelen style interaction occurs, with the adsorbed O_2 interacting with surface O•, forming O_3 on the surface before desorbing into the gas phase. Taking these two instances as an example, we can see that the same mechanism can proceed in very different manners, highlighting the importance of choosing the correct catalyst. This should help to bridge the gap between experimental and theoretical chemistry, and help to further increase O_3 yields as a result.

References:

1. Basiriparsa, J. Abbasi, M. J. Solid State Chem. 2012. 16. 1011
2. Christensen, P.A. Lin, W.F. Christensen, H. Imkum, A. Jin, J.M. Li, G. Dyson, C.M. Ozone:Sci and Eng. 2009. 31. 287
3. Wang, Y.H. Cheng, S. Chan, K.Y. Li, X.Y. J. Electrochem Soc. 2005. 11. D197
4. Christensen, P.A. Zakaria, K. Christensen, H. Yonar, T. J. Electrochem Soc. 2013. H405.
5. Gregory Gibson, Ashley Morgan, P. Hu, Wen-Feng Lin, Chemical Physical Letters, *Submitted*

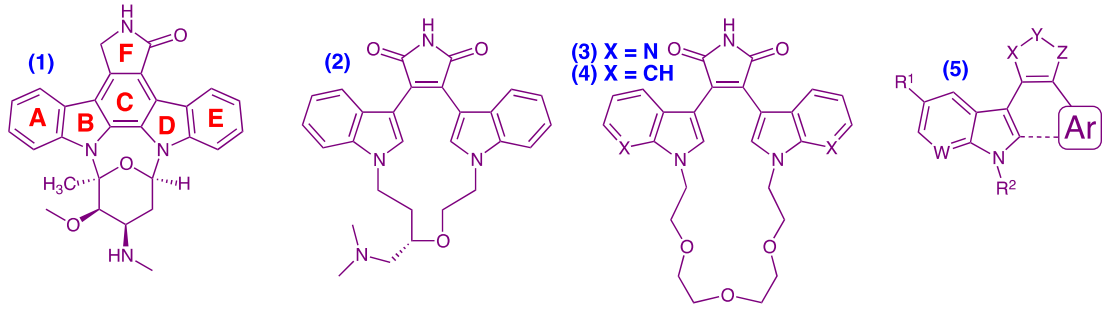
Email: ggibson04@qub.ac.uk

DESIGN, SYNTHESIS & EVALUATION OF NOVEL, FUNCTIONALISED INDOLES AS POTENTIAL INHIBITORS OF KINASE

O'Shea, K. D. and McCarthy F. O.
Analytical & Chemical Research Facility and Department of Chemistry, University College Cork.

Numerous disease states are associated with altered kinase activity and thus their inhibition is a subject of medicinal priority. Staurosporine **(1)** is a potent, non-specific inhibitor of PKC (IC_{50} = 2.7 nM) and is an important structural lead.[1] Kinases play pivotal roles in many cell-signaling pathways. Off target effects, especially those that eventually lead to undesirable side effects, are a clinical limitation making potent and specific inhibition a crucial goal. Ruboxistaurin **(2)**, a deconstructed bis-indolyl maleimide (BIM) version of staurosporine displays particular selectivity towards PKC-β and has entered clinical trials.[2] 7-Azaindole incorporation also pronounces selectivity further, as exemplified by **(3)**, a potent and selective inhibitor of GSK-3β (IC_{50} = 34 nM) in comparison to **(4)** where selectivity across a panel of 8 kinases is lost.[3] These findings alone show that it is possible to obtain some selectivity in action while preserving potency by exploiting discrete differences in the mode of ligand interaction in the protein active site.

We report on the design and synthesis of novel kinase inhibitory compounds through modification of general structure **(5)**. Replacement of the lactam/maleimide with a hydroxymaleimide F-ring, integration of the 7-azaindole bioisostere and pre-determined aryl components offer appealing templates with which to pursue further derivatives towards enhancement of enzyme-inhibitor contacts.[4,5] Functionalisation at the indole nitrogens and modification of the F-ring form an overarching theme from this. Biological evaluation has also been undertaken in collaboration with the NCI and Station Biologique, Roscoff, France.



1. Tamaoki, T. et. al., *Biochem. Biophys. Res. Commun.*, **1986**, 135, 397.
2. Brana M. et. al., *Bioorg. Med. Chem.*, **2006**, 14, 9.
3. Kuo, G. et. al, *J. Med. Chem.*, **2003**, 46, 4021
4. Pierce, L. T. et. al., *Eur. J. Med. Chem.*, **2006**, 14, 9.
5. Pierce, L. T. et. al., *Tetrahedron*, **2011**, 67, 25, 4601.

Investigation of the near-UV optical properties of secondary organic aerosols in an atmospheric chamber

Wilson, E.M[1,2]*; Kartigueyana, S[3] ; Prakash, N[4] ; Varma, R.M.[4]; Wenger, J.C[1,2]; Venables, D.S.[1,2]

1Centre for Research into Atmospheric Chemistry, University College Cork, Ireland
2Environmental Research Institute, University College Cork, Ireland
3University Paris-est Créteil (UPEC), Paris, France
4Department of Physics, National Institute of Technology Calicut, Kerala, India

In recent years, aerosol optical properties have received increasing interest due to the large uncertainties associated with their influence on the earth's radiative balance and hence on climate. Most studies of optical properties have focused on visible wavelengths where commercial instrumentation is available to measure particle scattering, absorption, and extinction. Owing to measurement challenges, the ultraviolet region has received less attention. However, this spectral region is where some particle constituents start to absorb strongly, with important implications for photochemical processes as well as the radiative balance in the troposphere. Incoherent broadband cavity-enhanced absorption spectroscopy (IBBCEAS) is an in situ spectroscopic technique that has proved useful in monitoring trace gases and aerosols in the atmosphere. IBBCEAS was developed in University College Cork [1] and has since been adopted by leading international atmospheric groups. Whereas other aerosol measurements are usually made at a few, discrete wavelengths, IBBCEAS can record broad, continuous optical property, making it suitable for application to aerosol studies [2-5]. In this work, we use an IBBCEAS spectrum with an unusually wide spectral range (340-410 nm) to study the optical properties of major biogenic and anthropogenic secondary organic aerosol (SOA) at short wavelengths.

Two types of SOA were studied in experiments carried out in a 4 m^3 atmospheric simulation chamber. SOA formed by the ozonolysis of α-pinene, a biogenic VOC, formed purely scattering particles, whereas SOA produced following photolysis of 2-nitrophenol, an anthropogenic species, were both scattering and absorbing. Aerosol extinction was measured using IBBCEAS and particle size distributions were monitored by a Scanning Mobility Particle Sizer (SMPS). Particle absorption was independently measured by dissolving filter samples in a methanol/water solution and quantifying the solution absorption using UV/vis spectroscopy. Using the IBBCEAS, the extinction, refractive index and scattering cross section were determined.

We gratefully acknowledge financial support from Science Foundation Ireland through awards 11/RFP/GEO3200 and 13/ISCA/2846.

References:

1. Fiedler, S.E., A. Hese, and A.A. Ruth, *Incoherent broad-band cavity-enhanced absorption spectroscopy.* Chemical physics letters, 2003. **371**(3): p. 284-294.
2. Washenfelder, R., et al., *Broadband measurements of aerosol extinction in the ultraviolet spectral region.* Atmospheric Measurement Techniques, 2013. **6**(4): p. 861-877.
3. Varma, R.M., et al., *Long optical cavities for open-path monitoring of atmospheric trace gases and aerosol extinction.* Applied optics, 2009. **48**(4): p. B159-B171.
4. Bluvshtein, N., et al., *A new approach for measuring the UV-Vis optical properties of ambient aerosols.* Atmos. Meas. Tech. Discuss., 2016. **2016**: p. 1-27.
5. Wilson, E.M., et al., *A novel, broadband spectroscopic method to measure the extinction coefficient of aerosols in the near-ultraviolet.* AIP Conference Proceedings, 2013. **1531**(1): p. 155-158.

Email: *eoin.wilson@umail.ucc.ie*

Session 2

BOOLE 3 & 4

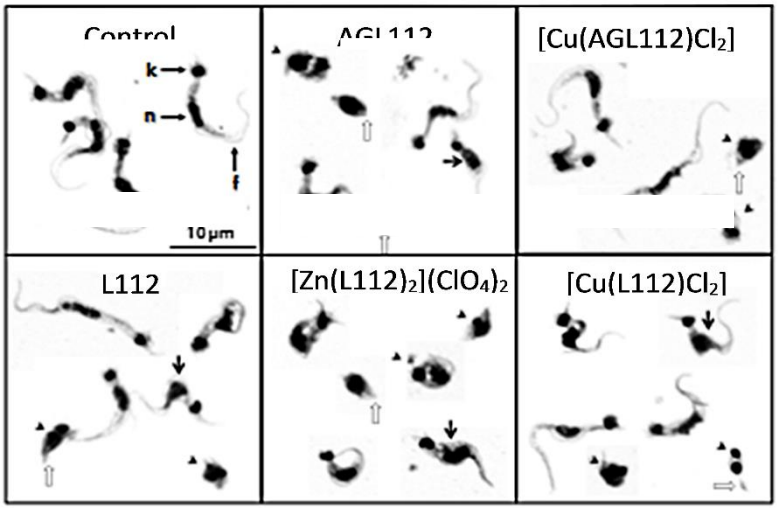
Parallel Sessions

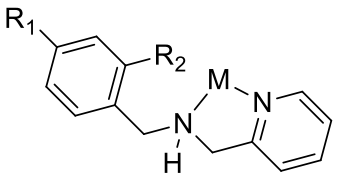
(Talks)

11.55 – 12.45 am

Synthesis, Characterization and *In Vitro* Anti-parasitic Activity of a Novel Family of Glycosylated Metallodrugs

Reddy A.* and Velasco-Torrijos T.
Maynooth University





Abstract:

Neglected tropical diseases (NTD) affect in excess of 1 billion people in the most impoverished areas of the world causing more than 500,000 deaths every year.[1] Of the major NTDs, the kinetoplastid parasite diseases visceral leishmaniasis and Chagas disease considered among the most challenging due to their high mortality rates and limited treatment options.[2]

A library of glycosylated chelators have been synthesized and several metal complexes have been obtained. Their ability to inhibit the growth of *T. Cruzi* and *L. amazonensis* have been evaluated and preliminary investigations into their toxicity towards mammalian cells have been carried out.

References:

1. *Working to overcome the global impact of neglected tropical diseases*. World Health Organization Geneva, Switzerland, 2010.

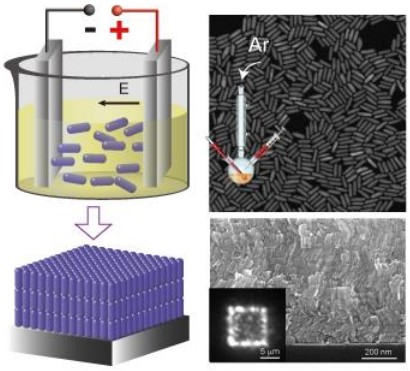
2. Cavalli, A.; Bolognesi, M. L., Neglected tropical diseases: multi-target-directed ligands in the search for novel lead candidates against Trypanosoma and Leishmania. *J Med Chem* **2009,** *52* (23), 7339-59.

Email: andrew.reddy@nuim.ie

Device Scale Assembly of Semiconductor Nanorods by Electrophoretic deposition

Liu, P.*; Ryan, K. M.

Department of Chemical and Environmental Sciences and Materials and Surface Science Institute (MSSI), University of Limerick, Limerick, Ireland



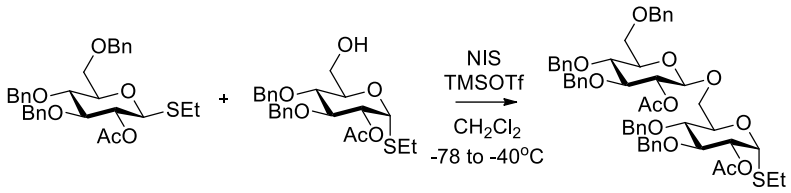
Abstract:

The organization of 1D nanocrystals into ordered assemblies is an area of significant interest in the field of nanotechnology as it allows supercrystals to be formed where the collective properties of the discrete components can be harnessed for bulk device application. In this study, we successfully assembled nanorods using electric fields into multilayer highly orientated films. This method can be applied to a range of materials from binary cadmium chalcogenides ($CdSe_xS_{1-x}$, CdSe) to quaternary copper chalcogenides nanorods (Cu_2ZnSnS_4), allowing complete control over orientational and positional order. We elucidate the effects of ligand, solvent chemistry, concentration, net particle charges, deposition time and applied voltage on the assembly formation. We further demonstrate the outstanding optical properties from a micrometer scale domain with the occurrence of lasing in the aligned sample and no lasing in the unaligned sample. Hence the electrophoretic deposition of nanorods provides a promising route for fabricating materials for optics, optoelectronics and photovoltaics by wet-processing techniques, and the knowledge gained from this study has the potential to provide the basis for creating low cost epitaxially grown semiconductor materials.

Email: Kevin.M.Ryan@ul.ie

CONFIGURATION-BASED ORTHOGONAL ACTIVATION OF THIOGLYCOSIDES

Smith, R.*; Zhu, X.
School of Chemistry, University College Dublin, Belfield, Dublin 4



The stability and diversity of thioglycosides has made these compounds one of the most widely used and versatile class of glycosyl donors in modern carbohydrate synthesis. Due to the low yields and poor selectivity associated with syntheses of α-*S*-glycosides using conventional approaches, research in this area has been heavily limited to β-configured compounds. Recent work in our group has helped to circumvent this issue by developing an efficient and stereoselective method for the synthesis of α-glycosyl thiols[1]. Our research has focused on exploring the potential applications of these thiols[2], particularly their ability to serve as straightforward precursors to their corresponding thioglycoside donors.

Landmark advances in donor reactivity modulation include Fraser-Reid's armed/disarmed concept[3], Demchenko's O-2/O-5 co-operative effect[4], and Bols' conformational arming strategies[5]. While these clearly demonstrate the power of protecting groups in altering donor strength, the influence of anomeric configuration remains relatively unexplored, particularly in relation to thioglycosides. It is well known that β-glycosides exhibit higher nucleophilicity due to increased dipolar repulsion with *O*-5, implying potentially faster reactions with glycosylation promoters. However, hypercojugation aspects of the anomeric effect result in a noticeably longer α-anomeric bond, indicating a greater likelihood of leaving group departure upon activation. Our recent work has investigated reactivity comparisons of a range of α- and β-thioglycosides with an aim developing a strategy for orthogonal donor activation based on anomeric configuration.

References:

1 Zhu, X .; Dere, R. T.; Jiang, J.; Zhang, L; Wang, X. *J. Org. Chem.* **2011**, *76*, 10187
2 a) Zeng, X.; Smith, R.; Zhu, X. *J. Org. Chem*. **2013**, *78*, 4165; b) Smith, R.; Zeng, X; Muller-Bunz, H.; X.; Zhu, X. *Tetrahedron Lett.* **2013**, *54*, 5348
3 Mootoo, D. R.; Konradsson, P.; Udodong, U.; Fraser-Reid, B. *J. Am. Chem. Soc.* **1988**, *110*, 5583
4 a) Mydock, L. K.; Demchenko, A. V. *Org. Lett.* **2008**, *10*, 2103; b) Premathilake, H. D.; Mydock, L. K.; Demchenko, A. V. *J. Org. Chem.* **2010**, *75*, 1095
5 Pedersen, C. M.; Nordstrøm, L. U.; Bols, M. *J. Am. Chem. Soc.* **2007**, *129*, 9222

Email: raymond.smith@ucdconnect.ie

Non-thermal plasma: a novel chemical decontamination tool

[1]Chaitanya Sarangapani*, [1]Paula Bourke, [1]PJ Cullen, [2]Finbarr O Regan [3]Patrice Behan

[1]*School of Food and Environmental Health, Dublin Institute of Technology Dublin 1*
[3]*School of Chemical & Pharmaceutical Sciences, Dublin Institute of Technology Dublin 1*
[2]*National Pesticide Residue Laboratory, Backweston, Kildare, Ireland*

Abstract

A significant amount of hazardous organic materials, mineral pollutants and pathogenic microorganisms are discharged into water sources, globally (1). Stringent regulations imposed for a mandatory clean water source and safe food drive the development of effective techniques to remove or degrade contaminants (2). In the present study, non-thermal plasma-induced degradation of chemical contaminants was investigated and characterised. Owing to the simultaneous initiation of physical effects (shock waves, UV/Vis light emissions) and chemical reactions (formation of reactive radicals, excited and active species), non-thermal plasma technology is reported as a sustainable low energy approach with no additional chemicals or heat required, thus presenting advantages over other advanced oxidation process (AOP's). The present study describes the discharge generation, demonstrates the efficacy of the resulting plasma generated species for organics removal and the characterisation of the degradation patterns.

Electrical measurements revealed the discharge operates in a filamentary regime. A stable discharge was found at the high voltages employed at the large discharge gap of 2.2 cm. Optical emission spectrometry results explained the presence of excited nitrogen species and relatively lower intensities of singlet oxygen and hydroxyl radical. The decontamination of pollutants by non-thermal plasma was characterized using model dyes (Methyl orange, bromothymol blue, and oil-red o). The effect generated in air on dye degradation was significant and kinetics followed pseudo-first order kinetic model. Non-thermal plasma significantly degraded organic content (COD, BOD, and TOC) of model dairy and meat effluents. A modified pseudo-first order kinetic model was proposed for organic degradation. The FTIR spectra of dairy and meat fat revealed the plasma induced effects were evident. These results were also confirmed by peroxide, iodine value and fatty acid profile. The oxidized products of fat were identified using GC-MS and degradation pathway was proposed.

Non-thermal plasma rapidly dissipated endocrine disruptors (EDC'S) in model food effluents, where effluent composition had a minor effect on degradation kinetics. The role of plasma species in degradation was studied using radical scavengers. Degradation kinetics were approximated using first-order rate equation. The degradation products were analysed by UHPLC-MS/MS, and the degraded EDC's were less toxic than the parent compound. Non thermal plasma treatment was effective for removal of pesticides in water and on fresh produce (removal rates >80%). The quality attributes of fresh produce after optimal treatment conditions were investigated. There was no significant effect on physical parameters such as color, texture and firmness. However, plasma treatment had minimal effect on chemical quality parameters. Overall, these results indicate that non-thermal plasma can be employed for chemical safety retention in wastewaters from the food manufacturing sector.

References:

1. Misra, N. N., Pankaj, S. K., Walsh, T., O'Regan, F., Bourke, P., & Cullen, P. J. (2014). In-package nonthermal plasma degradation of pesticides on fresh produce. *Journal of hazardous materials*, *271*, 33-40.
2. Sarangapani, C., Misra, N. N., Milosavljevic, V., Bourke, P., O'Regan, F., & Cullen, P. J. (2016). Pesticide degradation in water using atmospheric air cold plasma. *Journal of Water Process Engineering*, *9*, 225-232

Session 3

BOOLE 3 & 4

Parallel Sessions

(Flash Presentations)

12.45 am – 1.05 pm

The 'Smart' Needle – A Needle Integrated with an Impedance Sensor for Objective Nerve Localisation during Ultrasound Guided Peripheral Nerve Block

Helen, L.[1*]; O'Donnell, B.[2]; and Moore, E.[1]

[1] *Sensing and Separation Group, Chemistry Department and Life Science Interface Group, Tyndall National Institute, University College Cork, Ireland*
[2] *Department of Anaesthesia, Cork University Hospital, Cork, Ireland*

Abstract:

As the world of smart technology advances, insensate objects are being transformed to 'smart' devices by the application of sensors. Our research focuses on applying an impedance sensor to a hypodermic needle to create a 'smart' needle. This novel device will use bioimpedance to determine needle-to-nerve proximity for application in ultrasound guided peripheral nerve block (USgPNB) procedures. Bioimpedance data from the needle tip will allow for real-time tissue identification and thus provides the user with the exact needle tip location. For anaesthetists it will provide valuable information indicating needle contact with the nerve covering or dangerous needle position within the nerve. Introduction of this new technology to USgPNB will increase its safety, efficacy and training capacity thus increasing the use of the technique and reducing costs for the healthcare system, as it is a safer quicker alternative to general anaesthesia. The impedance sensor on the 'smart' needle is a miniaturised two electrode set-up. A prototype 'smart' needle, with electrodes directly integrated onto a commercially available needle, has been fabricated and characterisation is underway. Impedance values, using this 2nd generation 'smart' needle prototype, for different substances including saline solutions, phantom gelatine models and different tissue types in meat will be presented. Results have demonstrated that bioimpedance can be used to identify tissue type at the needle tip. The addition of 'smart' needle technology to USgPNB may provide a solution to a currently unmet clinical need.

Email: lisa.helen@tyndall.ie

Water Splitting at Transition Metal Oxide (TMO) Films in Alkaline Media - Cost vs. Activity

Browne, M.P* and Lyons, M.E.G
School of Chemistry and CRANN, Trinity College Dublin, Ireland.

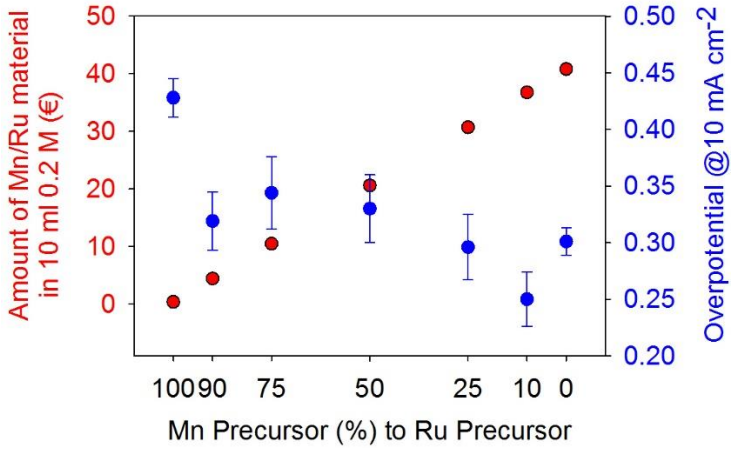


Figure 1: Cost vs. Activity for MnRu oxide OER electrocatalysts

Abstract:

Alkaline water electrolysis produces H_2 gas, which can be used as a fuel in H_2/O_2 fuel cells to generate power. The most energy intensive step in this reaction is the evolution of O_2 due to the large anodic overpotential of the Oxygen Evolution Reaction (OER).[1] Thus, understanding and optimising electrocatalysts for OER remains one of the grand challenges for both physical electrochemistry and energy science. For the OER in alkaline media, the best performing electrocatalysts are RuO_2, which exhibit the lowest OER overpotentials to date, but are expensive, making them impractical and uneconomical.[1] First row Transition Metal Oxides, show great promise as alternative materials for OER, due to their low costs.

In current literature, the OER catalytic activity of manganese oxide compounds display overpotentials between 0.74 - 0.49 V at a current density of 10 mA cm^{-2}.[2] Furthermore, when combined with other compounds this overpotential value further decreases. Pure and mixed Mn/Ru oxides are examined in this study. Several of the mixed materials were found to exhibit improved OER activity when compared with RuO_2, while lowering the cost of producing the catalyst, Figure 1.[2] These materials could therefore offer a competitive low-cost alternative to the already commercially available OER catalysts.

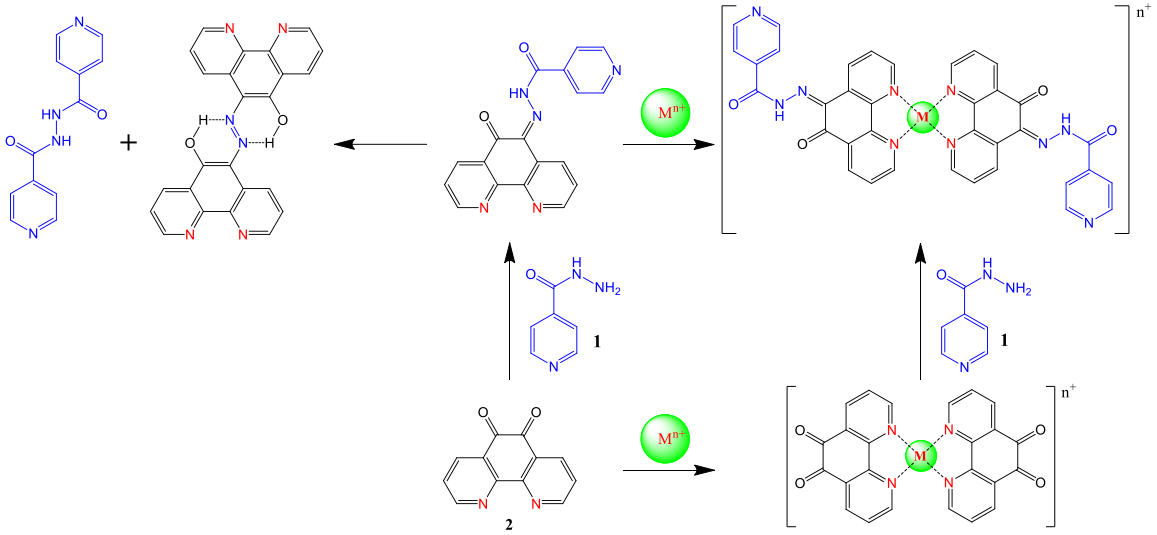
References:

(1) Lyons, M. E. G.; Doyle, R. L.; Fernandez, D.; Godwin, I. J.; Browne, M. P.; Rovetta, A. Electrochem. Commun. 2014, 45, 56.
(2) Browne, M. P.; Nolan, H.; Duesberg, G. S.; Colavita, P. E.; Lyons, M. E. G. ACS Catalysis 2016 .6, 4, 2408.

Email: Brownem6@tcd.ie

New Life for an Old Tuberculosis Drug

Ahmed, M.
Maynooth University



Abstract:

The World Health Organisation estimates that *ca.* 1.7 million people die annually from tuberculosis (TB), a disease caused by *Mycobacterium tuberculosis*.[1] The man-made pro-drug, isoniazid (INH, 1), has been successfully utilised in TB therapy since 1952, and is activated *in vivo* by a combination of the bacterial catalase-peroxidase, Kat G, and resident Mn(II) ions. However, many virulent strains of *M. tuberculosis* are now showing resistance to INH[2], and the focus of the present research involves derivatising INH with the powerful metal chelator, 1,10-phenanthroline-5,6-dione (dione, 2), and subsequently complex the resulting ligand to selected (Ag, Mn, Cu) metal centres (Fig.). Metal-free ligands and metal complexes will be ultimately screened for their anti-*M. tuberculosis* activity by collaborating laboratories.

References:

1 World Health Organisation. Tuberculosis Fact Sheet, 2014. Available from: http://www.who.int/mediacentre/factsheets/fs104/en/. Accessed: 7th May 2015.

2 Ramaswarny, S.V.; Reich, R. Dou, S.J. Jasperse, L. Pan, X. Wanger, A. Quitugua, T. and Gravis, E.A. *Antimicrob. Agents Chemother.*, 2003, 47 (4), 1241.

Email: MUHIB.AHMED.2011@mumail.ie

Novel miniaturized gold microelectrodes for electrochemical detection of hydrogen peroxide

[a*]Buk, V.; [b]Kelly, P.; [a]Twomey, K.
[a]*Tyndall National Institute, Lee Maltings, Dyke Parade, Cork.*
[b]*Teagasc Food Research Centre, Moorepark, Fermoy, Co.Cork*

Abstract:

The use of miniaturised electrodes in biosensor development provide many advantages which results in achieving high sensitivity in recognition of the target analytes [1]. As the size of the active area decreases to macro and nano dimensions, radial diffusion becomes dominant and mass transport enhances; resulting in a higher current density and increased the signal-to-noise ratio [2]. All of these unique features makes microelectrodes major materials in the development of electrochemical biosensors to improve electronic transduction [3].

In this work, a novel miniaturized biosensor based on a highly structured array of microelectrodes was developed to detect hydrogen peroxide from milk. To fabricate the microelectrode arrays standard microfabrication methods including UV photolithography was used. The process was fabricated at Tyndall National Institutes central semiconductor fabrication facilities [4, 5].

Pre-experiments were carried out using macroelectrodes for optimisation of the biosensor. Firstly, a mixture of known amount of chitosan (CS) and different amounts of multi walled carbon nanotubes (MWCNT) were electrodeposited onto the gold surfaces. As seen in Fig 1, 0.05 mg of MWCNT immobilized on the electrode surface exhibited the highest current response. Secondly, in order to determine the optimum one step-electrodeposition cycles of the CS- MWCNT mixture, different numbers of deposition cycles were applied at 0.15 to 0.20 V at a scan rate 20 mV/s. The amperometric results showed the most suitable deposition cycle number is 15 (Fig.2). Current investigations are being carried out on the use of PAMAM (Polyamidoamine) dendrimers and gold nanoparticles (AuNPs) to determine the most suitable platform for hydrogen peroxide sensing.

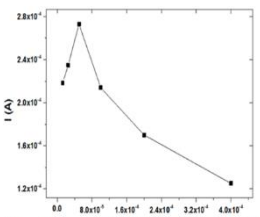


Figure 1. Amount of MWCNT in electrochemical cell (g)

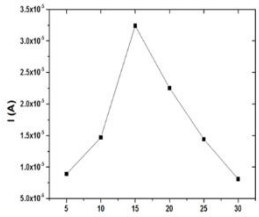


Figure 2. Number of chitosan deposition cycles

References:

[1] Yeh, J.I., Du, S., Xia, T., Lazareck, A., Kim, J.-H., Xu, J., Nel, A.E., 2007. Coordinated Nanobiosensors For Enhanced Detection: Integration Of Three Dimensional Structures To Toxicological Applications. *ECS Transactions* 3 (29), 115–126.

[2] Bard, A.J., Faulkner, L.R., 1980. Electrochemical Methods: Fundamentals and Application. *John Wiley & Sons, New York*, NY, p. 208.

[3] Ma H., Sun J., Zhang Y., Bian C., Xia S., Zhen T., 2016. Label-free immunosensor based on one-step electrodeposition of chitosan-gold nanoparticles biocompatible film on Au microelectrode for determination of aflatoxin B_1 in maize. *Biosensors and Bioelectronics* 80: p. 222–229.

[4] Twomey, K., et al., Fabrication and characterization of a miniaturized planar voltammetric sensor array for use in an electronic tongue. *Sensors and Actuators B: Chemical*, 2009. 140(2): p. 532-541.

[5] Twomey, K., et al., Fabrication and Characterization of a Test Platform Integrating Nonporous Structures with Biochemical Functionality. *Sensors Journal, IEEE*, 2015. 15(8): p. 4329-4337.

Email:vuslat.buk@tyndall.ie

Development of Bespoke Metal Complexes for Cellular Targeting

Kitteringham, E.*; and Griffith, D.M.
[1] *Department of Pharmaceutical and Medicinal Chemistry, Royal College of Surgeons in Ireland, Dublin, Ireland*

Abstract:

Metal complexes provide an excellent platform for the rational design of drug candidates through the prediction and control of the pharmacodynamics and pharmacokinetics of such compounds. These complexes have an advantage over traditional organic drugs due their increased 3D structural geometry and stereoisomers which may improve binding and access within cells.(1) Although in its infancy, the rational design of metallodrugs for specifically targeting well-characterised protein binding sites within cells by improved access through unique 3D binding space and selective interaction has enormous potential. (2, 3, 4)

Much research has been undertaken to identify novel biomolecular targets for anti-cancer therapeutic exploitation. HSP70-1 is overexpressed in many cancers and is associated with cancer progression, chemotherapeutic resistance and poor prognosis as it is thought to provide cancer cells with a survival advantage by conferring protection against apoptosis, influencing senescence and inhibiting autophagy and HSP90 client protein function. (4, 5, 6)

Although metals have a long history in medicine many of the so called essential metals have poorly understood biochemistries. Metals themselves can act as imaging agents by their own photochemical properties or by the attachment of ligands. (2, 3) By tracking these complexes in the cell through rational design improved understanding of the metals cellular trafficking and therapy can be obtained.

This work focuses on the development of metal complexes that exhibit therapeutic, diagnostic and a combined theranostics effect as a potential alternative treatment for colorectal cancer that could have intrinsic or acquired resistance. The inhibition of HSP70-1 is one avenue being investigated in this study. A summary of synthetic chemistry and analytical results to date will be described.

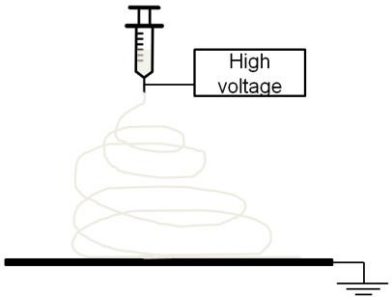
References:

1 Meggers, E. *Chem.Comm*., **2009**, 9, 1001.
2 Gaynor D. and Griffith D.M., *Dalton Trans*, **2012**, 41, 13239.
3 Chellan, P. and Sadler P.J., Phil. Trans. R. Soc. A, **2015**, 373(2037).
4 Allardyce, C.S. and Dyson, P.J., *Dalton Trans*, **2016**, 45, 3201.
5 Juhasz, K.,; Lipp, A. M.; Nimmervoll, B. et al., *Cancers*, **2014**, 6(1), 42.
6 Murphy, M.E., *Carcinogen*, **2013**, 34 1181.

Email: eolannkitteringham@rcsi.ie

Electroactive Bioresorbable Materials for Tissue Engineering Scaffolds

Heffernan, M.*, O'Reilly, E.
Department of Chemical and Environmental Sciences,
Materials and Surface Science Institute,
University of Limerick.



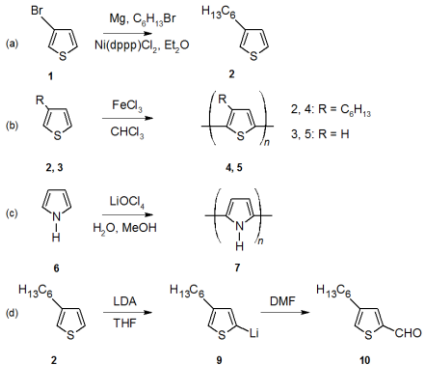


Figure 1: Typical experimental set-up used for electrospinning of PCL solutions.

Scheme 1: Synthetic pathway followed in the preparation of a number of conducting polymers and thiophene based oligomeric units.

Abstract:

Naturally occurring scaffolds consist of 3D networks made up of protein nanofibers that provide mechanical support for cells to proliferate and maintain their differentiated functions.[1] In order to create a synthetic scaffold, it must be analogous to this in terms of chemical composition, morphology and mechanical strength. Studies have illustrated the in-vivo compatibility of conducting polymers (CPs) with biological molecules[2]. Their flexibility, physicochemical properties and ability to electrically stimulate and control cell growth[3] make CPs suitable candidates for biomedical applications. This work focuses on the synthesis and characterization of CPs, preparation of biodegradable heterocyclic oligomeric units and the fabrication of 3D organic scaffolds via electrospinning of biodegradable polymeric materials.

References:

1. Kadler, K. E., Holmes, D. F., Trotter J. A., Chapman J. A. Biochem. J., 1996, 316 (1) p. 1-11.
2. Wang, X., Gu, X., Yuan, C., Chen, S., Zhang, P., Zhang, T., Yao T., Chen F., Chen, G. J. Biomed. Mater. Res. Part A, 2004, 68 (3), 411–22.
3. Balint, R., Cassidy, N. J., Cartmell, S. H. Acta Biomater. , 2014, 10 (6), p. 2341-53.

Email: Maria.Heffernan@ul.ie

In Silico Determination of Dioxygen Addition to a (Cp*)Ru(II) β-diketiminate Complex

Phillips, A. D. and Gaynor, B.*
UCD School of Chemistry, University College Dublin

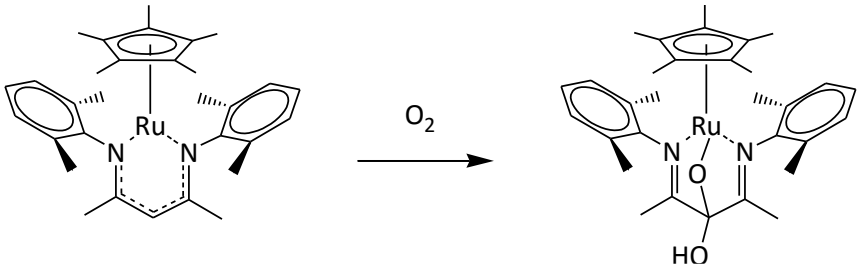


Fig 1: Reaction scheme for oxygen addition to a neutral (Cp*)Ru(II) β-diketiminate Complex

Abstract:

In recent years the Phillips' research group has carried out investigations in to methods of safe hydrogen storage technology. A class of complexes that have shown promising activity in this area are the (η^6-arene)Ru(II) β-diketiminates. These complexes have shown the ability to carry out thermally reversible heterolytic cleavage of dihydrogen and promote subsequent hydrogenation of C-C π-bonded molecules.[1] A complex was designed that uses the anionic η^5-Cp* ligand in place of an η^6-arene ligand.[2] This altered complex does not display the same activity as the arene based systems. However, it does undergo an unusual rearrangement with dioxygen when exposed to a non-protected environment. It is found that the dioxygen bond is cleaved during the reaction and a bridge is formed by a single oxygen atom between the Ru centre and the β-C centre of the β-diketiminate ligand. Moreover, a hydroxyl group is formed at the β-C position of the β-diketiminate ligand. It has also been found that an acidified analogue of this complex undergoes a similar but seperate rearrangement upon exposure to unprotected conditions, in this case an oxo-bridge is formed, the Cp* ligand is deprotonated and there is a formal loss of a water molecule. The purpose of this computational investigation was to determine, using DFT analysis, the most likely mechanisms by which this rearrangement occurs.

References:

[1] Schreiber, D. F.; Connor, C. O.; Grave, C.; Mu, H.; Scopelliti, R.; Dyson, P. J.; Phillips, A. D. Organometallics 2013, 32, 7345–7356.

Email: brian.gaynor@ucdconnect.ie

Design and Evaluation of New Biomaterials to Treat Fungal Infection

Newman, G.*; Deasy, M.; Fleming, A. and Kavanagh, K.
Institute of Technology Tallaght

Abstract:

Implant infection is emerging as a critical medical problem. Implant-associated infections pose serious complications in orthopaedic surgery. Current statistics indicate that infection is responsible for up to 15% of implants associated with orthopaedic trauma. The current market value figures ($16 billion in the US) and projections point to an upward increase in implant production worldwide. Some of the largest medical device industries are based in Ireland and are fighting to keep pace with infection preventative solutions for their products. Implants with antimicrobial surfaces have been developed to try and address infection, but the emphasis has been on antibacterial surfaces to date.

While antimicrobial drugs demonstrate significant activity against infection in solution, this activity diminishes when immobilised in a material/surface.[1] Few studies have focussed on antifungal surfaces. According to the Centre for Disease Control and Prevention (USA 2012), *Candida Albincans* is the 4th most common Healthcare Associated Infection (HAI), arising from infection via medical implants such as catheters, central lines etc. Azole compounds are well recognised for their antifungal activity. Activity has been shown to increase when coordinated to Cu(II) or Ag(I) ions in a complex. The aim is to make new implant materials, incorporating anti-fungal compounds, and evaluate their effectiveness in vitro.

Tetrazoles are synthetic organic heterocyclic compounds that are unknown in nature. They consist of a 5-membered ring containing four nitrogen atoms and one carbon atom plus one hydrogen atom.

We have synthesized a series of novel tetrazole compounds to date, and some metal complexes. Preliminary biological evaluation of these compounds and complexes have been carried out in NUI Maynooth prior to surface adherence and the results from this work will be presented in this presentation.

References:

1 Deelstra, J.; Neut, D. and Jutte, P. *J Arthroplasty*, 2013, 28 (2), 374

Email: gemma.newman@postgrad.ittdublin.ie

Session 4

BOOLE 3 & 4

Parallel Sessions

(Talks)

2.15 – 4.30 pm

Selective aliphatic/aromatic organogelation controlled by the side-chain protection of serine amphiphiles

Jessica Ramos* and Trinidad Velasco-Torrijos
Maynooth University, Maynooth, Co. Kildare, Ireland.

Abstract:

Supramolecular organogels formed through the self-assembly of small molecules into structured three-dimensional networks are versatile "smart materials"[1,2] which are finding numerous applications in fields as diverse as waste management[3,4], drug delivery and tissue engineering[5], to name but a few. Fmoc-serine lipoamino-acids were found to selectively induce the gelation of either aromatic or aliphatic hydrocarbon solvents depending on the presence or absence of protecting groups in the serine side chain. Extension of the chain length of the lipoamino-acid (from C-14 to C-18) decreases the selectivity observed for the shorter chain homologues. The organogels obtained are thermoresponsive, mouldable and capable of self-healing. In addition, the lipoamino-acids studied are efficient phase selective gelators in biphasic mixtures of water/organic solvent and efficiently remove water soluble polluting dyes from the aqueous phase.

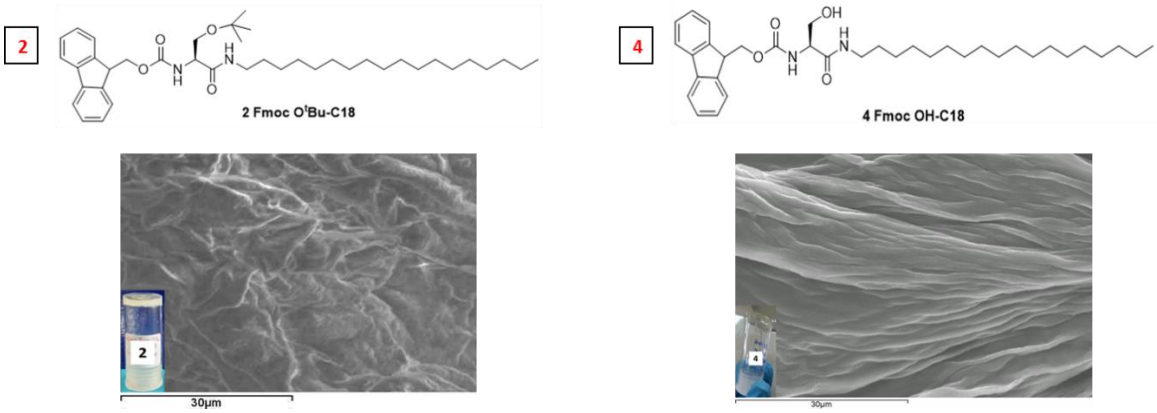


Figure 1: SEM images of xerogels from lipoamino-acids **2** and **4** formed by the drop-cast method

References:

1 Hirst, A. R.; Escuder, B.; Miravet, J. F.; Smith, D. K. *Angew. Chem. Int. Ed.* 2008, *47*, 8002.
2 Aida, T.; Meijer, E. W.; Stupp, S. I. *Science* 2012, *335*, 813.
3 Okesola, B. O.; Suravaram, S. K.; Parkin, A.; Smith, D. K. *Angew. Chem. Int. Ed.* 2015, n/a.
4 Yao, X.; Wu, S.; Chen, L.; Ju, J.; Gu, Z.; Liu, M.; Wang, J.; Jiang, L. *Angew. Chem.* 2015, *127*, 9103.
5 Skilling, K. J.; Citossi, F.; Bradshaw, T. D.; Ashford, M.; Kellam, B.; Marlow, M. *Soft Matter* 2014, *10*, 237.

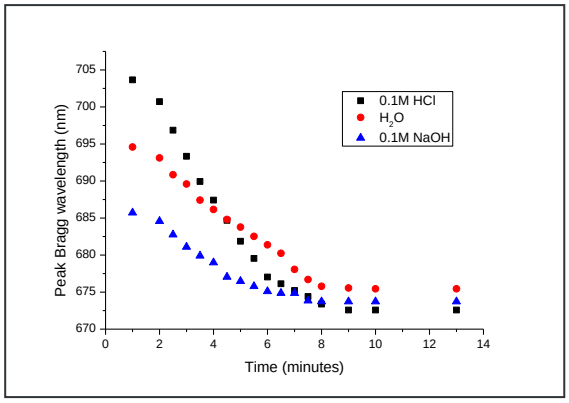
Email: jessica.ramos.2014@mumail.com

An organic-inorganic composite designed for pH-driven optical detection by combination of chitosan and colloidal silica

Ryan, C.C.*; Bardosova, M. and Pemble, M.E.
Tyndall National Institute, University College Cork

Abstract:

A chitosan-tetraethylorthosilicate-silica (Chi-TEOS-SiO_2) composite was synthesised by combining two separate entities with different sensitivities.
The first entity, chitosan, forms a versatile interpenetrating polymer network (IPN) when combined with TEOS as a cross-linker. The flexibility and pH-sensitivity of the IPN is provided by chitosan with TEOS contributing to the mechanical strength. The IPN was studied with respect to varying molecular weight of chitosan and varying TEOS cross-linker concentration. The second entity is a colloidal photonic crystal constructed of spherical silica particles in the range of 250-350nm. This size range allows for analysis in the visible region of the electromagnetic spectrum as the particle diameter is analagous to Bragg diffracted wavelength. The organic-inorganic composite is formed by embedding the photonic crystal in the IPN. Essentially, the ordered colloidal SiO_2 is surrounded by the pH-sensitive chitosan structure. Therefore, as the chitosan network swells in reaction to external pH the SiO_2 crystal lattice will also swell. The final composite efficiently exhibits this proof of concept as the Bragg diffracted wavelength of the photonic crystal shifts as a function of pH, as displayed in the graph below [1].



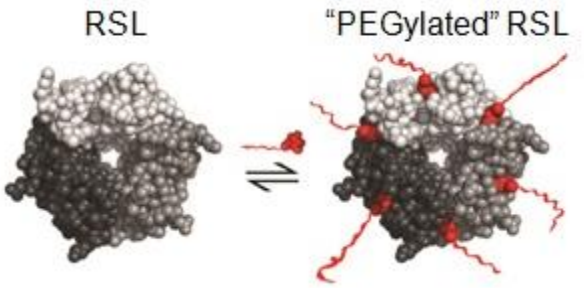
References:

1. Ryan, C., et al., *Silica-based photonic crystals embedded in a chitosan-TEOS matrix: preparation, properties and proposed applications.* J. Mater. Sci., 2016. **51**(11): p. 5388-5396.

Email: catherine.ryan@tyndall.ie

Lectin–Glycopolymer Interactions as a Route to Noncovalent PEGylation

Antonik, P.M.[a,b]*; Eissa, A.M.[c]; Round A.R.[d]; Cameron, N.R.[c]; and Crowley, P.B.[a];
[a]*School of Chemistry, National University of Ireland Galway, Galway, Ireland*
[b]*Teagasc Food Research Centre, Ashtown, Dublin 15, Ireland*
[c]*Department of Chemistry, University of Durham, Durham, United Kingdom*
[d]*European Molecular Biology Laboratory, Grenoble University Grenoble, France*



Abstract:

PEGylation, the covalent attachment of polyethylene glycol (PEG) to proteins, is a widely used method to improve pharmacokinetics.[1,2] The disadvantage of this technique is that the PEG chains can reduce biological activity of the protein.[1,2] Reversible, noncovalent PEGylation has the potential to overcome this limitation of the current technology.

RSL (~29 kDa trimer) is a hexavalent fucose-binding lectin from the bacterium *Ralstonia solanacearum*[3] that we characterized recently by NMR spectroscopy.[4] Here, we describe the interactions of RSL with a fucose-capped polyethylene glycol (Fuc-PEG). Using a combination of NMR spectroscopy, small angle X-ray scattering (SAXS), size exclusion chromatography (SEC) and native gel electrophoresis we demonstrate that RSL and Fuc-PEG form a high molecular weight protein-polymer "Medusa complex". Moreover, we show that the assembly is reversible and the protein-polymer affinity is in the µM range.

References:

1 Caliceti, P.; and Veronese, F. M. *Adv. Drug Deliv. Rev.* **2003**, *55*, 1261
2 Kontos, S.; and Hubbell, J. A. *Chem. Soc. Rev.* **2012**, *41*, 2686
3 Kostlanova, N.; Mitchell, E. P.; Lortat-Jacob, H.; Oscarson, S.; Lahmann, M.; Gilboa-Garber, N.; Chambat, G.; Wimmerova, M.; and Imberty, A. *J. Biol. Chem.*, **2005**, *280*, 27839
4 Antonik, P.M.; Volkov, A.N.; Broder U.N.; Lo Re, D.; van Nuland, N.A.J.; and Crowley, P.B. *Biochemistry*, **2016**, *55*, 1195

Email: p.antonik1@nuigalway.ie.

Design and characterization of amperometric glutamate biosensors

Ford, R.,* Quinn, S.J. and O'Neill, R.D.
School of Chemistry, University College Dublin, Belfield, Dublin 4

Abstract:

A biosensor consists of two main functional components: a sensitivity element to detect the target analyte, and a selectivity layer to reject interference molecules. An amperometric glutamate (Glu) biosensor was designed, where the former was glutamate oxidase (GluOx) and the latter was poly-*ortho*-phenylenediamine (PoPD) which was electro-deposited on the electrode surface (1 mm long Pt cylinder, 125 µm diameter). PoPD is permeable to hydrogen peroxide (HP, the enzyme-generated signal molecule) and non-permeable to ascorbic acid[1] (AA, the most significant interference species in biological tissues and fluids[2]).
Various modifications of the Pt electrode were made to enable the biosensor to be suitable in an *in-vivo* environment: inclusion of a permselective PoPD layer; deposition of GluOx by dip evaporation; the introduction of enzyme stabilisation agents, such as polyethyleneimine (PEI)[3]; and enzyme crosslinkers such as poly(ethylene glycol) diglycidyl ether (PEGDE); see **Fig.1**. Non-conducive nanoparticles were also included in some biosensor designs in an attempt to increase the surface loading of GluOx.

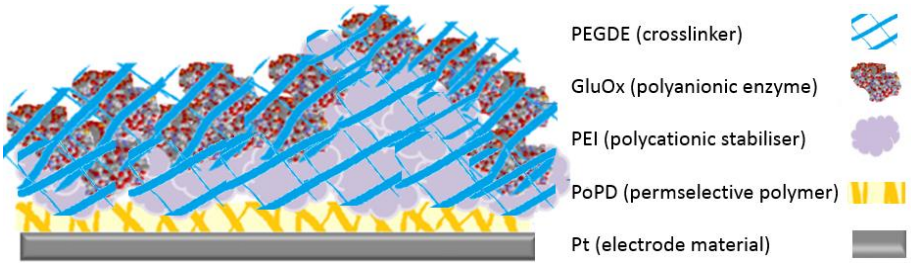


Figure 1: Schematic of our biosensor design, showing the electro-deposited polymer PoPD on the Pt electrode, the immobilisation of glutamate oxidase (GluOx, 140 kDa) over polyethyleneimine (PEI, 750 kDa), and the crosslinking of PEGDE with amine groups located on the GluOx and PEI molecules.

To date the best configuration of biosensor components is Pt with electro-deposited PoPD, dip coated twice with 1% PEI, 5 dips of 400 U mL^{-1} GluOx, and crosslinked with 0.1% PEGDE, which can be represented as $Pt/PoPD/PEI_2/GluOx_5/PEGDE$.

References:

1 Killoran, S.J. and O'Neill, R.D. *Electrochim. Acta*, 2008, 53, (24), 7303
2 Kennedy, R.T. Thompson, J.E. and Vickroy, T.W. *J. Neurosci. Methods*, 2002, 114, (22), 39
3 McMahon, C.P. Rocchitta, G. Serra, P.A. Kirwan, S.M. Lowry, J.P. and O'Neill, R.D. *Analyst* 2006, 131, (1), 68.

Email: Rochelle.ford@ucdconnect.ie

Pt Anticancer Compounds; Targeting HSP70-1

*McKeon, A[1]; Platts, J[2] and Griffith D[1].

[1]*Centre for Synthesis & Chemical Biology, Department of Pharmaceutical and Medicinal Chemistry, The Royal College of Surgeons in Ireland, Dublin 2.*[2]*Theoretical and Computational Chemistry Group, Cardiff University, UK.*

Abstract:

Colorectal cancer is a major cause of death and disease worldwide. Current treatment options depend on the stage of the cancer but can generally include surgery, radiotherapy and chemotherapy. Oxaliplatin, a platinum (Pt)-based compound, plays a very important and well documented role in treating colorectal cancer [1]. The cytotoxicity of Pt drugs is attributed to multiple mechanisms but primarily their ability to enter cells, hydrolyse and covalently bind DNA, causing the formation of DNA adducts. These events can lead to DNA damage responses and ultimately programmed cell death, apoptosis. The clinical efficacy of Pt drugs is limited however by drawbacks, such as toxicity, but primarily by the high incidence of chemoresistance (intrinsic or acquired) [2]. Since many colorectal cancers are intrinsically resistant to platinum-based therapies there is an urgent need to develop novel and innovative therapeutic strategies for combating colorectal cancer. The HSP70 family of heat shock proteins are highly conserved molecular chaperones whose expression is increased by cells in response to a variety of cellular stresses. HSP70 is overexpressed in colorectal cancer, amongst other cancers, and is associated with cancer progression, chemotherapy resistance and poor prognosis, as it is thought to provide cancer cells with a survival advantage [3]. HSP70 is therefore an exciting and legitimate anti-cancer target.

Consequently, we wish to develop novel platinum HSP70 inhibitor complexes as potential treatments for colorectal cancer. A summary of our research to date will be described.

References:

1 Kasparkova, J.; Vojtiskova, M.G.; Natile, G.V. and Brabec V. *J. Chem. Eur.* 2008; 1300.
2 Piccart, M.J.; Lamb, H. and Vermorken J.B. *Ann. Oncol.* 2001; 1195.
3 Murphy, M. E. *J. Carcinog*. 2013; 1181.

Email: aoifemckeon@rcsi.ie

Fluorescence Emission Properties of Triazine Fluorophores in Micelle and Protein Solutions: *A Comparison*

Ryder, A.G. and Kyne, M. *
National University of Ireland, Galway.

Abstract:

Fluorophores, based on a 1,2,3-triazine core with substituted aryl groups, showed interesting emission properties and have many potential biomedical applications (1). Here we studied in detail the photophysical behaviour of 5-methoxycarbonyl-5-(N-phenylformimidoyl)-2,4,6-triphenyl-2,5-dihydro-1,2,3-triazine (pTr), with a view to understanding how it might be used as a protein label. In most organic solvents, pTr had a strong absorbance band at 310 nm (S_2 excitation) with a weaker band at ~400 nm (S_1 excitation). Fluorescence was complex with three emission bands centered at 520 nm when excited at 405 nm. These bands originated from three vibrationally accessible geometrical conformers (g_0, g_1, and g_2). Inter-conversion between these conformers occurs in the excited state, and was relatively insensitive to solvent type (2).

The pTr fluorophore was very hydrophobic and its behaviour in more simple aqueous environments (*e.g.* buffer solutions) was difficult to reproducibly measure. A range of non-ionic, anionic, and cationic surfactants were therefore used to solubilize the triazine and to serve as a simple model for its behaviour in the hydrophobic pocket of a protein. For non-ionic and cationic surfactant solutions, the shape and position of each individual fluorescence emission band changed very little while the fluorescence anisotropy and lifetime increased, indicating that while the fluorophore was located within the micelle, the changed environment did not have a very large effect on emission properties (3). The triazine's incorporation within the micelle was also confirmed by energy transfer studies using tetramethylrhodamine isothiocyanate (TRITC) as an acceptor. In the anionic surfactant, pTr emission was found to be partially quenched, and this was ascribed to an electron exchange/Dexter interaction with the charged head group.

The interaction between Bovine Serum Albumin (BSA) and pTr was investigated under various conditions of pH and protein-fluorophore ratios. The interaction was rapid, but the emission spectrum did not change significantly, apart from a hypsochromic shift of ~22.5 nm. This mimicked the small blue shift observed on going from aqueous solution to a micelle environment (except SDS where a bathochromic shift was present). The pTr fluorescence lifetime decreased upon protein binding and was most pronounced at longer wavelengths. The pTr-BSA construct had an average fluorescence lifetime ($405_{ex}/550_{em}$) of 5.72 ns which was much shorter than that observed in micelles. There was an increase in fluorescence anisotropy, but compared to micelle environments pTr seemed to be less rigidly confined by the protein. In conclusion, we suspect that pTr is not contained within the hydrophobic cavity of BSA but rather located on its exterior where it is subject to quenching and solvent effects.

References:

1. Butler, R. N.; Fahy, A. M.; Fox, A.; Stephens, J. C.; McArdle, P.; Cunningham, D.; Ryder, A. G. *The Journal of Organic Chemistry*, 2006, 71 (15), 5679.
2. St. Mart, D.; Togashi, D.M.; Stephens, J.; Burke, L.A.; Ryder, A.G.: *in preparation*.
3. Kyne, M., and Ryder, A.G. *in preparation*.

Email: m.kyne2@nuigalway.ie

Session 5

BOOLE 3 & 4

Parallel Sessions

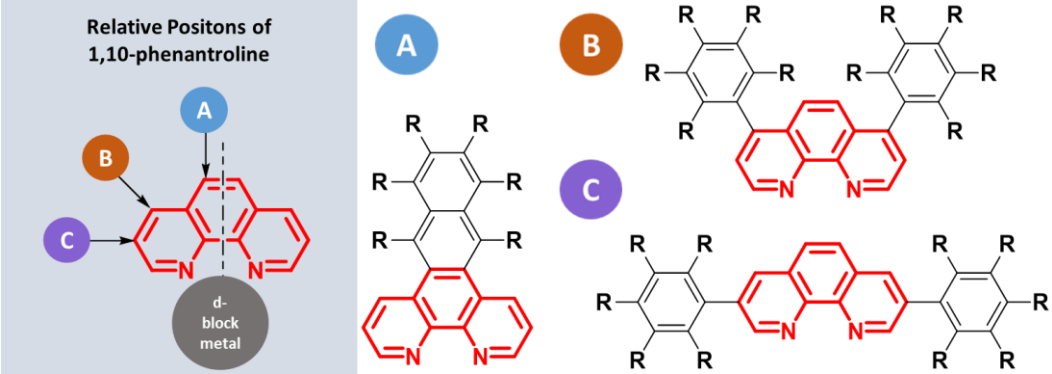
(Talks)

4.00 – 4.50 pm

UCC
University College Cork, Ireland
Coláiste na hOllscoile Corcaigh
Department of Chemistry

Synthetic Potential; Large Poly-Phenyl Ligands Derived from 1,10-Phenanthroline

Conway-Kenny, R.;* Draper, S.M.
University of Dublin, Trinity College



ABSTRACT:

Photosensitisers containing π-electron ligand systems have found use in a diverse range of fields including photocatalysis,[1] biological imaging,[2] phosphorescent organic light emitting diodes (PHOLEDS),[3] electron transfer relays[4] and photocatalytic hydrogen production.[5] Large π-ligand systems can be derived from a base unit of 1,10-phenanthroline (phen), and may be split into two classes; those containing freely rotating poly-phenyl rings and those containing π-expansive fused ring systems. Despite the extensive number of potential uses for ligands of this kind, only a limited number of large phen-containing systems are present in the current literature. There is an opportunity therefore to develop novel synthetic strategies to extensively to fill this gap. In addition, phen-based ligand systems provide optimally located nitrogen atoms for the rapid and facile bidentate metalation of d-block metals. This synthetically-driven work presents new routes to a considerable library of novel complexes for application in all the related fields of coordination and supramolecular chemistry.

REFERENCES:

1 Rau, S.; Schäfer, B.; Gleich, D.; Anders, E.; Rudolph, M.; Friedrich, M.; Görls, H.; Henry, W.; Vos, J. G. *Angew. Chem. Int. Ed. Engl.* 2006, *45* (37), 6215.

2 Gill, M. R.; Thomas, J. A. *Chem. Soc. Rev.* 2012, *41* (8), 3179.3 Tsuboyama, A.; Iwawaki, H.; Furugori, M.; Mukaide, T.; Kamatani, J.; Igawa, S.; Moriyama, T.; Miura, S.; Takiguchi, T.; Okada, S.; Hoshino, M.; Ueno, K. *J. Am. Chem. Soc.* 2003, *125* (42), 12971.4 Flamigni, L.; Collin, J.-P.; Sauvage, J.-P. *Acc. Chem. Res.* 2008, *41* (7), 857.5 Paul, A.; Das, N.; Halpin, Y.; Vos, J. G.; Pryce, M. T. *Dalton Trans.* 2015, *44* (22), 10423.

Email: smdraper@tcd.ie

Effect of the Presence of MEA on CO_2 Capture Ability of Superbasic Ionic Liquids

McCrellis, C. *; Taylor, S.F.R.; Jacquemin, J.; Hardacre, C.
Queen's University Belfast

Abstract:

Recently Ionic Liquids (ILs) composed of a tetra-alkyl-phosphonium cation paired with a superbasic anion have been reported to exhibit equimolar CO_2 absorption with efficient CO_2 capture and release under ambient conditions.[1] Further investigation of these promising results has been carried out including a study of the effect of the superbase anion structure on the CO_2 capture and release.[2] These ILs show only small changes in viscosity after reaction with CO_2 unlike amino acid based ILs, for example, which have been studied extensively. To date, literature studies have focussed on CO_2 capture under dry conditions; however, for the application of CO_2 capture from flue gas it is important to understand the effect of water on the CO_2 uptake. In this work, the effect of water on the CO_2 capture of $[P_{66614}][124Triz]$, $[P_{66614}][PhO]$, $[P_{666,14}][Bentriz]$, $[P_{666,14}][123Triz]$ and $[P_{666,14}][Benzim]$ has been evaluated showing that depending on the anion, water can have a positive or negative effect on the CO_2 uptake. As well as water the effect of the presence of monoethanolamine (MEA) on the CO_2 uptake and release in these superbasic ILs was studied. Recent literature studies show that MEA has no promotional effect on the CO_2 uptake in many ionic liquids; however, it does have an effect on the rate of uptake.[3,4] The latter is due to the decrease in viscosity on the addition of the co-solvent. In contrast, in this work, we have shown that the presence of MEA has the ability to enhance the CO_2 capture for two of the superbasic ionic liquids suggesting that both the IL and MEA are working synergistically.[5]

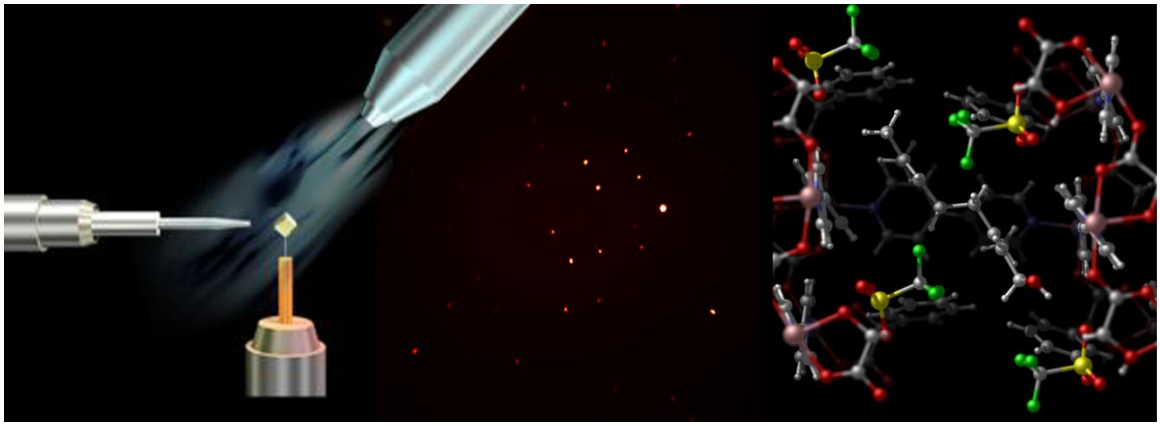
References:

1 Dai *et al*. Angew. Chem. Int. Ed. 2011, 50, 4918
2 Taylor *et al*. J. Solution Chem. 2015, 44, (3), 511
3 Camper *et al*. Ind. Eng. Chem. Res. 2008,47, 8496
4.Baj *et a*l. J Chem Technol Biotechnol. 2013, 88, 220
5 McCrellis *et al*. *J. Chem. Eng. Data*. 2016, 61, (3), 1092

Email: cmccrellis01@qub.ac.uk

A Chiral Crystalline Sponge

Zhang, S.-Y. *; Zaworotko, M.J.
Department of Chemical & Environmental Science, University of Limerick, Limerick, Republic of Ireland



Abstract:

X-ray crystallography is an essential tool to determine molecular structure. However, this technique requires high quality single crystals of target compound. Crystalline sponge method[1] has the capability of analysing the compond of interest without its crystalline form. We have prepared a chiral crystalline sponge base upon mandelate (man) and 4,4'-bipyridine (bpy) ligands, $[Co_2(S\text{-man})_2(bpy)_3](OTf)_2 \cdot$guest. The cationic frameworks exhibit 1D chiral channels with maximum dimensions of 8.0 Å × 8.0 Å. The pore chemistry is such that chiral surfaces lined with triflate anions and phenyl groups order the guests within the framework lattice. The host chiral crystalline sponge absorbs geraniol within its channels that can be determined by X-ray diffraction. Our chiral crystalline sponge method requires extremely low quantity as 17μg of geraniol. Moreover, the robust chiral crystalline sponge crystallized in lower space group with confined channels has rendered itself as a candidate for practical application of determining various targets. The results of these experiments will be presented and discussed.

References:

1 Inokuma, Y.; Yoshioka, S.; Ariyoshi, J.; Arai, T.; Hitora, Y.; Takada, K.; Matsunaga, S.; Rissanen, K.. and Fujita, M. *Nature*, 2013, 495 (7442), 461.

Email: xtal@ul.ie

Real-time Imaging of Lysosomal Disruption with a pH Responsive NIR Fluorophore

Cheung, S.; Grossi, M. and O'Shea, D.F.
Royal College of Surgeons in Ireland

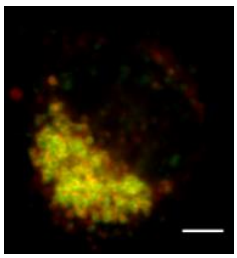


Fig.1 GFP labelled lysosomal membrane (green) surrounding NIR fluorophore "on" at pH5 (red)

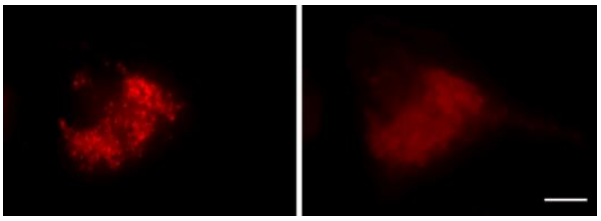


Fig.2 Selectively stained lysosomes (left), and prodigiosin induced deacidification of lysosomes (right).

Abstract:

Near infrared (NIR) fluorescence is a useful tool for probing biological processes as it allows for real time imaging. Our group has developed NIR fluorophores which are fluorescently silent at pH7, but in acidic lysosomes (pH~5) have a strong emission (1). This permits highly selective staining of lysosomes in living cells and in real time imaging of their disruption. Prodigiosin is a bacterial pigment which is a highly potent anion receptor that has been reported to selectively de-acidify lysosomes (2). This process causes apoptosis, which is triggered by a low cytosolic pH. As part of my PhD a new method to 4D-image in real-time lysosome disruption by prodigiosin has been developed which allows visualization of all the key stages of the process from lysosome de-acidification, to cytosol acidification and cell entry into apoptosis.

.

References:

1 Murtagh, J., Frimannsson, D. O., & O'Shea, D. F. (2009). *Organic Letters*, (2009), *11*(23), p5386
2 Gale, P. A, Pérez-Tomás, R. & Quesada, R., (2013) *Accounts of Chemical Research*,(2013), 46(12), p2801

Email: shanecheung@rcsi.ie

Session 6

BOOLE 3 & 4

Parallel Sessions

(Flash Presentations)

4.50 – 5.10 pm

Synthesis of Novel Magnetic Catalysts

Ensar Mulametovic and Gráinne Hargaden

School of Chemical and Pharmaceutical Sciences, Dublin Institute of Technology, Kevin Street, Dublin 8

Abstract:

Chiral catalysts used in asymmetric transformations have become an essential component of modern day organic synthesis. Through the use of organometallic and bio/organocatalysis, many highly efficient synthetic methods have been developed which provide academically and industrially desirable, enantioenriched products. However, while there are many asymmetric catalysts that offer remarkably high enantioselectivity as well as efficiency, problems associated with reusability of these catalysts has still not been sufficiently addressed. Therefore, in order to obtain greater applicability of asymmetric catalysts in industry, the development of easily recyclable chiral catalysts is of key importance.

Due to their rigid modular structure and ability to bind metals through a nitrogen lone pair, chiral oxazoline-containing catalysts have shown significant efficacy in many important organic transformations. While the use of such catalysts on an industrial scale may be uneconomical due to poor methods of recovery, immobilisation of such catalysts onto inorganic magnetic supports such as iron oxides is desirable. For this reason, the development of a range of chiral oxazoline-proline ligands as well as their inorganic magnetic carriers has been undertaken.

A small library of halogenated oxazoline-proline ligands were prepared possessing *iso*-propyl, *tert*-butyl, phenyl and benzyl substituents on the oxazoline component of the ligand, respectively, offering good to high yields of 67-85%. Additionally, initial work on iron oxide particle formation, coating and functionalisation will be presented.

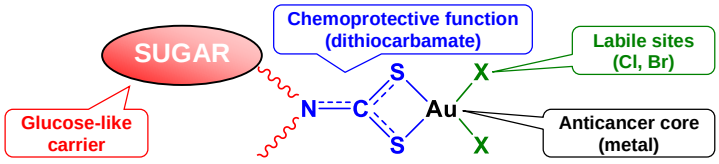
Email: Ensar.Mulametovic@dit.ie

Recent Developments of Gold(III) Dithiocarbamato Glycoconjugates for the Targeted Metal-Based Anticancer Chemotherapy

Pettenuzzo, A.*; Ronconi L.*
School of Chemistry, National University of Ireland, Galway, University Road, Galway, Ireland

Abstract:

Some gold(III)-dithiocarbamato complexes have recently shown promising antitumor activity, both *in vitro* and *in vivo*, together with negligible systemic and organ toxicity, [1,2] although selective tumor targeting is still a major issue.
In order to maximize the impact on cancer cells and minimize side-effects, our latest approaches focus on complexes with tumor targeting properties provided by the coordination of biologically-active ligands.
In such perspective, rapidly dividing tumor cells requires higher amounts of nutrients and energy for their fast proliferation, and glucose is no exception. Accordingly, such increased demand of glucose by fast-proliferating cancer cells makes it very attractive to selectively target tumor sites. In particular, tailored glucose-like substrates can be conjugated to chemotherapeutics (including metal-containing anticancer agents) so as to attain the site-specific delivery of drugs into the affected tissues.[3]
Starting from the rationale behind our research work, the main results achieved to date are here summarized, focusing on the development of gold(III)-dithiocarbamato glycoconjugates for the targeted chemotherapy.



Acknowledgments
Financial support by National University of Ireland Galway (CoS Scholarship) and Irish Research Council (Government of Ireland Postgraduate Scholarship) is gratefully acknowledged.

References:

1 Nagy, E.M.; Ronconi, L.; Nardon, C. and Fregona, D. *Mini-Rev. Med. Chem.*, 2012, 12, 1216.
2 Ronconi, L.; Nardon, C.; Boscutti, G. and Fregona, D. *Perspective Gold(III)-Dithiocarbamato Anticancer Therapeutics: Learning from the Past, Moving to the Future* in *Advances in Anti-Cancer Agents in Medicinal Chemistry – vol. 2* (Prudhomme M). Bentham Science Publishers, Bussum, 2013, pp 130.
3 Pettenuzzo, A.; Pigot, R. and Ronconi, L. *Metallodrugs*, 2015, 1, 36.

Email: a.pettenuzzo1@nuigalway.ie

68th Irish Universities Chemistry Research Colloquium
June 23rd & 24th, 2016.

UCC University College Cork, Ireland Coláiste na hOllscoile Corcaigh | Department of Chemistry

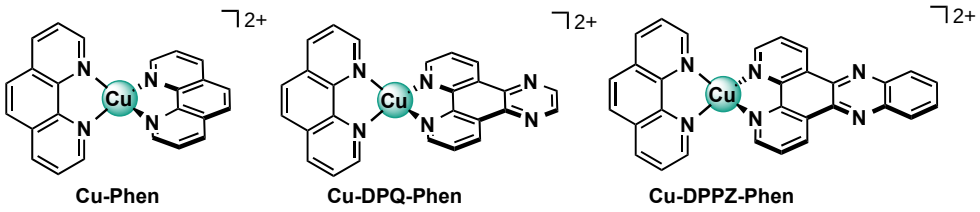
DNA Oxidation Profiles of Copper Phenanthrene Chemical Nucleases

Molphy Z.,* Slator C. and Kellett A.

School of Chemical Sciences and National Institute for Cellular Biotechnology, Dublin City University

Abstract:

The deleterious effects of metal-catalyzed reactive oxygen species (ROS) in biological systems can be seen in a wide variety of pathological conditions including cancer, cardiovascular disease, ageing, and neurodegenerative disorder. On the other hand, however, targeted ROS production in the vicinity of nucleic acids – as demonstrated by metal-activated bleomycin – has paved the way for ROS-active chemotherapeutic drug development. This work present results obtained from range of new inorganic materials as potential anticancer agents using high-throughput biophysical experiments developed within the Kellett research group. These assays have enabled us to successfully probe the oxidative nuclease activity and redox properties of a range of copper(II) developmental therapeutics $[Cu(DPQ)(phen)]^{2+}$ (Cu-DPQ-Phen), $[Cu(DPPZ)(phen)]^{2+}$ and (Cu-DPPZ-Phen) with results being compared directly to Sigman's reagent $[Cu(phen)_2]^{2+}$ (phen = 1,10-phenanthroline; DPQ = dipyridoquinoxaline; DPPZ = dipyridophenazine).[1–3]



Scheme 1. Molecular structures of the copper(II) complex cations examined in this study.

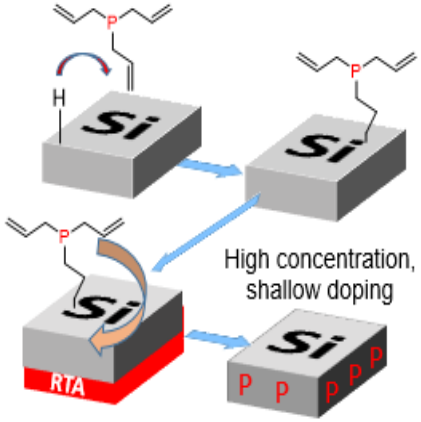
References

1 Molphy Z., Prisecaru A., Slator C., Barron N., McCann M., Colleran J., Chandran D., Gathergood N. and Kellett A., *Inorg. Chem.*, 2014, **53**, 5392.
2 Molphy Z., Slator C., Chatgilialoglu C. and Kellett A., *Front. Chem.*, 2015, **28**.
3 Sigman D. S., Graham D. R., Aurora V. D. and Stern A. M., *J. Biol. Chem.*, 1979, **254**, 12269.

E-mail: zara.molphy2@mail.dcu.ie

Monolayer doping of Si and $InGa_{0.53}As_{0.47}$ substrates and devices for future CMOS applications

O'Connell, J* and Holmes, J.D.
Materials Chemistry and Analysis Group, Department of Chemistry, University College Cork, Ireland



Abstract:

Monolayer doping has shown promise as a solution for ultra-shallow doping of traditional semiconductors such as Si[1,2] and Ge[3] and upcoming replacement materials such as InGaAs. This allows for the continued scaling-down of devices present in all of our electronic devices. Presented is a summary of recently published group work carried out on the controlled nanoscale doping of Si and InGaAs via an organic functionalisation route.

References:

1 **O'Connell J**, Verni G A, Gangnaik A, Shayesteh M, Long B, Georgiev Y M, Petkov N, McGlacken G P, Morris M A, Duffy R and Holmes J D **2015** Organo-arsenic Molecular Layers on Silicon for High-Density Doping **ACS Appl. Mater. Interfaces** 7 15514–21

2 **O'Connell J**, Collins G, McGlacken G P, Duffy R and Holmes J D **2016** Monolayer Doping of Si with Improved Oxidation Resistance **ACS Appl. Mater. Interfaces** 8 4101–8

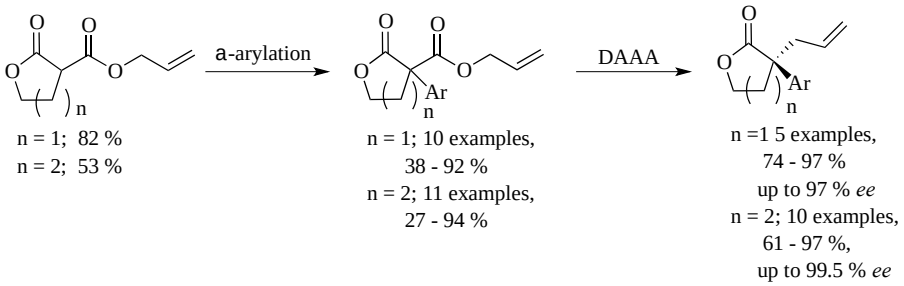
3 Long B, Alessio Verni G, **O'Connell J**, Holmes J, Shayesteh M, O'Connell D and Duffy R 2014 Molecular Layer Doping: Non-destructive doping of silicon and germanium **Proceedings of the International Conference on Ion Implantation Technology** (Portland) pp 1–4

Email: j.holmes@ucc.ie

Catalytic asymmetric synthesis of sterically hindered α-allyl-α-aryl lactones

James, J.*; Guiry, P. J.

Centre for Synthesis and Chemical Biology, School of Chemistry, University College Dublin, Belfield, Dublin 4, Ireland



Abstract:

The generation of quaternary stereocentres is a significant challenge in synthetic organic chemistry. However, methods that are both mild and enantioselective in forming these stereocentres are extremely desirable given their prevalence in a wide range of natural products with important structural and biological properties.[1] Pd-catalysed decarboxylative asymmetric allylic alkylation (DAAA) has become one of the most successful approaches for the construction of enantioenriched α-quarternary carbonyl compounds.[2,3] As part of the focus on the enantioselective synthesis of sterically hindered α-aryl carbonyl compounds within our research group,[4,5,6] we aimed to develop Pd-catalysed DAAA for sterically hindered α-aryl lactones.

Lead-mediated α-arylation of the β-oxo-allylester was used as the key step to synthesise the substrates for catalysis. Optimisation studies for DAAA were conducted using the 2,4,6-trimethoxyphenylated 6-membered lactone. Using (*R,R*)-ANDEN-phenyl Trost as the chiral ligand, enantioselectivities of up to 99.5 % *ee* and 97 % *ee* were achieved for the six-membered and five-membered lactones, respectively. This synthetic route allows for the simple modification of the aryl groups, giving access to important structural motifs.

References:

1 Mohr, J. T. and Stoltz, B. M. *Chemistry – An Asian Journal.* 2007, *2*, 1476.
2 Behenna, D. C. and Stoltz, B. M. *J. Am. Chem. Soc.* 2004, *126*, 15044.
3 Trost, B. M. and Xu, J. *J. Am. Chem. Soc.* 2005, *127*, 2846.
4 Carroll, M. P.; Müller-Bunz, H. and Guiry, P. J. *Chem. Commun.* 2012, 48, 11142.
5 Doran, R. and Guiry, P. J. *J. Org. Chem.* 2014, *79*, 9112.
6 Doran, R.; Carroll, M. P.; Akula, R.; Hogan, B. F.; Martins, M.; Fanning, S. and Guiry, P. J. *Chem. Eur. J.* 2014, *20*, 15354.

Email: jinju.james@ucdconnect.ie

Nanowire-based, Label-free Electrochemical Detection of Bovine Respiratory Disease Pathogens in Serum

Creedon, N.[a]*; Montrose, A.[a]; Sayers, R[b] and O'Riordan, A[a].
[a] *Tyndall National Institute, University College Cork, Dyke Parade, Cork, Ireland.*
[b] *Teagasc, Moorepark, Fermoy, Cork Ireland.*

Abstract:

Bovine viral diarrhoea virus (BVD) is a global disease with severe financial implications for the Bovine beef and dairy industries. A key challenge to the virus eradication is that the current turnaround time for analysis of serological samples using ELISA, a lab-based diagnostic process, is more than 72 hours. This allows for uncontrolled spread of the virus within a herd and possible transmission to herd cohorts. Rapid identification of BVD pathogens is now critical for herd protection and prevention of costly outbreaks. Consequently, new diagnostic devices, suitable for on-farm analysis, that deliver rapid and early identification of animal disease states, are required.

To address this, an on-chip fully integrated nanowire based electrochemical immunosensor was developed for the detection of BVD in buffer and serum. Capture biomolecules e.g. recombinant antigens, corresponding to viral surface proteins are covalently immobilized via a carboxylic terminated polymer electrodeposited onto a single nanowire. Electrochemical characterization including electrochemical impedance spectroscopy and cyclic voltammetry is performed for the detection of immune responses to the viral protein. The nanowire-based immunosensor allows the specific serological detection of BVD antibodies (10 µg/mL, 20 min) and clearly discriminates between positive and negative infected bovine sera obtained from cattle.

This electrochemical biosensor technology provides rapid, label-free and cost-efficient sensing capability in a compact size, and clearly shows the potential for immunoassay applications with a view to developing portable point-of-care devices for on-farm diagnosis or therapeutic monitoring in animal health applications.

Email: niamh.creedon@tyndall.ie

Poster Session

Kampus Kitchen Hall

5.10 – 6.10 pm

Counterfeit Product Identification using Broadband Acoustic Resonance Dissolution Spectroscopy (BARDS)

Alfarsi, A.; Ní Chrónín,E.; MC Sweeney, S.; Keating, J.J and Fitzpatrick, D.
* Department of Chemistry, University College Cork, Ireland

Abstract

The objective of this work is to demonstrate the potential of a new platform technology called BARDS to discriminate between genuine and counterfeit products, e.g., Cialis, Levitra, Viagra and anti-malarial tablets. A simple dissolution test, taking <3 minutes, is shown to provide reproducible changes in the compressibility of the solvent which is unique to a particular tablet formulation. The changes in compressibility are measured through corresponding changes in acoustic resonant frequencies of the dissolution vessel which are mechanically induced using a magnetic follower. Counterfeit formulations are shown to produce significantly different acoustic profiles compared to genuine products.

Authentic and counterfeit tablets of the products were measured in duplicate as received using a BARDS spectrometer. A dissolution vessel containing 25 mL of 0.1M HCl was induced to resonate using a magnetic stir bar. Background resonances are observed for 30 seconds before the auto-addition from a tipper of a half tablet. The dissolution medium rapidly dissolves the half tablet which results in outgassing and reproducible changes in the compressibility of the solution which in turn alters the resonant frequencies of the vessel.[1-5] The method harnesses an acoustic effect reported notably by F.S. Crawford.[5]

Time vs frequency plots were obtained during the dissolution of the tablets using dedicated software. Genuine products are shown to yield reproducible and consistent data indicative of formulations produced under high specifications. However, counterfeit tablets produce different acoustic profiles which are less reproducible which indicates poor blend uniformity of the formulations. Different frequency minima in the spectra, as well as the time taken to return to steady state of the system are all indicators as to whether the material being tested is authentic pharmaceuticals or counterfeits when compared to the control of the genuine drug. Further work is required to produce a larger statistical dataset of counterfeit products (n=30).

BARDS was shown to differentiate between genuine and counterfeit samples of all prescription drug products. This represents a rapid ‘low tech’ approach to screen suspect products using genuine product as a reference control.

References

1. Fitzpatrick, D., J. Krüse, et al. (2012). "**Principles and Applications of Broadband Acoustic Resonance Dissolution Spectroscopy (BARDS): A Sound Approach for the Analysis of Compounds.**" Analytical Chemistry 84(5): 2202-2210.
2. Fitzpatrick, D., R. Evans-Hurson, et al. (2013). "**The relationship between dissolution, gas oversaturation and outgassing of solutions determined by Broadband Acoustic Resonance Dissolution Spectroscopy (BARDS).**"Analyst 138(17): 5005-5010.
3. Fitzpatrick, D., E. Scanlon, et al. (2012). "**Blend uniformity analysis of pharmaceutical products by Broadband Acoustic Resonance Dissolution Spectroscopy (BARDS).**" International Journal of Pharmaceutics 438(1-2): 134-139.
4. Fitzpatrick, D., R. Evans-Hurson, et al. (2014). "**Rapid Profiling of Enteric Coated Drug Delivery Spheres via Broadband Acoustic Resonance Dissolution Spectroscopy (BARDS).**" Analyst 139(5): 1000-1106.
5. Crawford, F.S., (1981) ‘**The hot chocolate effect’** American Journal of Physics, 50(5), 398-404.

Email: 111220141@umail.ucc.ie

Platinum(IV) complexes with a histone deacetylase inhibitor in axial position as potent antitumor agents

Awatif Almotairy [a], Diego Montagner [b], Andrea Erxleben [a]
[a]School of Chemistry, National University of Ireland, Galway, Ireland.
[b]School of Chemistry ,National University of Ireland, Maynooth, Ireland.

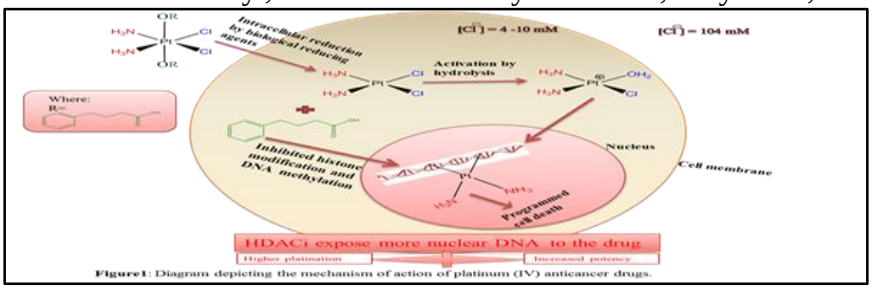


Figure1: Diagram depicting the mechanism of action of platinum (IV) anticancer drugs.

Abstract:

The most attractive advantage of platinum(IV) prodrugs is their reduced toxicity and higher stability compared to the corresponding Pt(II) species. Pt(II) analogues play an important role in cancer chemotherapy and has become the gold standard of treatment of many cancers [1]. However, the main problem associated with Pt(II) complexes and cisplatin analogues in particular, are the poor solubility and the high toxicity. The chlorido ligands of cisplatin readily undergo hydrolysis, and cisplatin and its analogues can bind to different biomolecules before reaching the final target namely the nuclear DNA. One strategy to overcome these side effects is to develop a Pt(IV) species (octahedral) which provides superior stability. Inside the cell, Pt(IV) complexes are reduced to the corresponding Pt(II) species with the release of the axial ligands [2].The primary objective of this study is to synthesise Pt(IV) complexes based on well-known anticancer drugs namely cisplatin, carboplatin and oxaliplatin with 4-phenylbutyric acid (4-PBA) in axial position. The ligand is a histone deacetylase inhibitor which displays anti-cancer activity, in addition to inhibiting cell proliferation and inducing the process of apoptosis. This new series of Pt(IV) prodrugs will be activated via reduction inside the cell, releasing two important bioactive molecules (cisplatin and 4-PBA) simultaneously. These molecules that possess different mechanisms of action, will improve the anti-proliferative properties (Figure1). The complexes have been characterized by various methods. The reduction of the complexes by ascorbic acid was studied by monitoring the release of the bioactive ligand by HPLC and the reduction potentials were determined by cyclic voltammetry in order to determine structure/activity correlations. The cytotoxic activity was evaluated in various cancer cell lines.

References:

[1] T. Boulikas, M. Vougiouka, Oncol. Rep. 11 (2004) 559–595.
[2] D. Montagner, S.Q. Yap, W.H. Ang, Angew.Chem.125 (2013) 12001-12005.

Email: a.almotairy1@nuigalway.ie

The Crystallisation of Active Pharmaceutical Ingredients (APIs) onto Excipient Matrices

Raquel Arribas-Bueno, Barry Murphy, Vivek Verma, Clare Crowley, Peter Davern, Sarah Hudson & Kieran Hodnett

Synthesis and Solid State Pharmaceutical Centre, Department of Chemical and Environmental Sciences, Materials and Surface Science Institute, University of Limerick

Abstract:

Chadwick et al [1] previously showed that crystallisation of acetaminophen (AAP) in the presence of dispersed excipient particles ('quasi seeds') such as β-D-Mannitol (β-D-Man) and α-Lactose monohydrate (α-LMH) resulted in specific API-excipient molecular interactions which led to a reduction in the induction time for the nucleation of AAP. This project is therefore concerned with understanding and optimising API-excipient interactions to promote API nucleation and growth on and/or in the excipient particles with the aim of enhancing API dissolution rates. This approach may prove advantageous insofar as primary heterogeneous nucleation may increase nucleation rates leading to a reduction in crystal size. Additionally, crystallisation in the presence of excipients may also streamline downstream processing by potentially obviating the need to mill API batches, and could improve solids handling properties.

As schematically illustrated in Figure 1, the interaction of APIs (paracetamol (AAP), carbamazepine (CBMZ) and fenofibrate (FFR)) with excipient particles (β-D-Man, α-LMH, α/β-Lactose (α/β-Lac), δ- D-Mannitol (δ-D-Man), microcrystalline cellulose (MCC) and carboxymethyl cellulose (CMC)) has been examined under various process conditions and the isolated solids characterised.

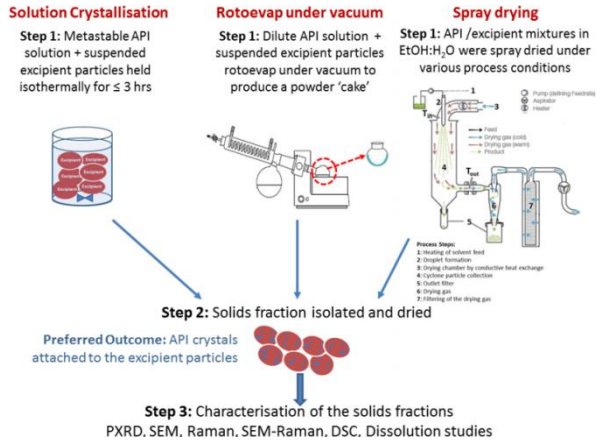


Figure 1: Schematic illustration of the processes performed

References:

1 Chadwick, K. et al. Crystal Growth & Design 2012, 12, 1159

Email: Raquel.ArribasBueno@ul.ie

DNA Sensor as a Tool to Investigate the Interactions between DNA and Bioinorganic Compound

Banasiak, A.*; Cassidy, J.; Colleran, J.
Dublin Institute of Technology

Abstract:

The aim of this research project is to electrochemically investigate the interactions between DNA and bioinorganic compounds, used as candidates for cancer therapeutics and as anti-microbial agents, with a view to elucidating the mode of action of these drugs.
Bioinorganic compounds interact with DNA through covalent binding or non-covalent binding: groove binding or intercalation. Additionally, some of the bioinorganic compounds after binding to DNA can participate in Fenton-like reaction (with H_2O_2) in the cell that leads to a creation reactive oxygen species. Radicals cause serious DNA damages *inter alia* strand breakage or oxidation of bases in the DNA strand. DNA damage can result in premature cell death.
A DNA biosensor is an electrode with DNA immobilized on the surface. Interactions between immobilized DNA and any molecules, such as, DNA strands or bioinorganic compounds, can be interpreted through an electrochemical current response.
The critical step in the project is to immobilise DNA oligonucleotide layers onto the electrode surfaces in the optimal way. Good surface is necessary to provide high reactivity, accessibility and stability of the immobilized DNA. When the DNA layer is dense the redox behaviour of the bioinorganic compound is visible only if the compound interacts with the DNA biosensor. During the redox cycling of bioinorganic molecules at DNA biosensors, electrons need to be transferred to and from the electrode surface to the compound. Oxidation or reduction of the metal centre is thought to occur via a long range electron transfer mechanism - DNA base pairs behaving as the electron conduit.
These simple devices can deliver information about changes in DNA structure caused by drug interaction. These data should allow the identification of effective drug candidates, or those with a suitable therapeutic mode of action. Variation of the DNA oligonucleotide sequences will help to determine any structure or region specific DNA-drug interactions. The DNA biosensors are immersed in solution containing the bioinorganic compound of choice. Changes in the measured current response of the sensor, in the presence of a bioinorganic compound, can provide information about type of binding interaction and about the DNA cleavage mechanism (if any) of that compound.

References:

1 Brett, A.M.O. *Encyclopedia of Sensors*, 2006, vol. 10, 1
2 Fojta, M. *Electroanalysis*, 2002, vol. 14, 1449

Email: anna.banasiak@mydit.ie

Probing the Magnetic and Photophysical Properties of Iron(III) Spin Switches

Barker, A.*; Cowley, M.; Sundaresan, S.; Salley, D.; Müller-Bunz, H.; Morgan, G. G.
School of Chemistry, University College Dublin, Belfield, Dublin 4, Ireland.

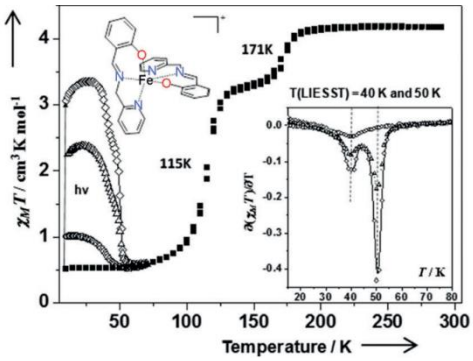


Figure: X_mT versus T iron(III) complex showing the LIESST effect at 10 K. Thermal relaxation after (○) irradiation at 647.1nm during 2 h, irradiation at 830 nm during 3 h (△) and 12 h (◇). Structure of the complex cation is shown above the plot. The first derivative in the insert shows a double step relaxation curve. Transition temperatures are indicated.

Abstract:

Thermal spin state switching in some transition metal complexes of iron, manganese and cobalt have been widely studied, with a strong focus on the magnetic properties.[1,2] Of equal importance are the photophysical properties in both the solid state and in solution, in some instances this can lead to long lived excited states in crystalline samples[3] termed Light Induced Excited Spin State Trapping (LIESST). The LIESST mechanism of Fe(II) (d^6), whereby two electrons are excited and spin flipped by a single photon, has been extensively debated in recent years.[4,5] Much less studied is the LIESST mechanism in Fe(III) (d^5).[6] The phenomenon is unknown in Mn(III) (d^4) and Co(II) (d^7). We present here recent magnetic and photophysical properties of some iron(III) spin crossover complexes and rationalise the difference between them.

References:

1. Gütlich, P.; Gaspar, A.; Garcia, Y.; *Beilstein J. Org. Chem.* 2013, **9,** 342.
2. Halcrow, M. A.; *Chem. Soc. Rev*. 2011, **40**, 4119.
3. Hauser, A.; *Top. Curr. Chem.* 2004, **234,** 155.
4. Auböck, G.; Chergui, M.; *Nature Chemistry.* 2014, **7,** 629.
5. Zhang, W.; Alonso-Mori, R.; Bergmann, U.; Bressler, C.; Chollet, M.; Galler, A.; Gawelda, W.; Hadt, R. G.; Hartsock,R.W.; Kroll, T.; Kjær, K. S.; Kubicek, K.; Lemke, H. T.; Liang, H, W.; Meyer, D. A.; Nielsen, M. M.; Purser, C.; Robinson, J. S.; Solomon, E. L.; Sun, Z.; Sokaras, D.; Van Driel, D. B.; Vanko, G.; Weng, T-C.; Zhu, D.; Gaffney,K.J; *Nature*, 2014, **509**, 345.
6. Bertoni,R.; Lorenc, M.; Laisney, J.; Tissot, A.; Moréac, A.; Matar, S. F.; Boillot, M. L.; Collet, E.; *J. Mater. Chem. C*. 2015, **3**, 7792.

Email: andrew.barker@ucdconnect.ie

CZTSSe Solar Cells Fabricated from CZTS Nanorods

Bree, G*[†]; Coughlan, C[†]; Just, J.[‡]; Unold, T.[‡] and Ryan, K.M.[†]
University of Limerick[†], Helmholtz Zentrum Berlin[‡]

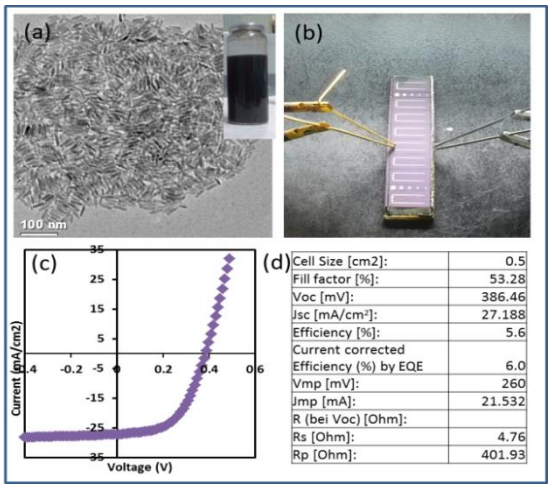


Figure 1: (a) TEM image of CZTS Nanorods, (b) the completed solar cell undergoing testing, (c) the resulting IV (current-voltage) curve, and (d) the measured parameters

Abstract:

Solar photovoltaic cells based on the material Copper Zinc Tin Sulfide/Selenide (CZTS/Se) have great potential to further reduce the cost of solar energy. Cell efficiencies for this technology have increased rapidly over recent years, reaching a current record of 12.6%[1]. In UL & HZB we have fabricated a 6% efficient cell using a nanoparticle method. The rod-shaped CZTS nanoparticles (as seen in Figure 1a) are synthesised by a colloidal hot injection method[2]. This method is advantageous as it does not require vacuum based processes (unlike e.g. sputtering/evaporation), while maintaining excellent performance[3]. The solar cell was formed by depositing a 2µm layer of the CZTS nanorods onto a molybdenum substrate using doctor blading, and annealing at high temperature (500C) in the presence of selenium vapour. CdS, ZnO & ITO were then deposited sequentially to form the p-n junction and top contact. Figure 1c shows the IV curve of the 6% cell, while Figure 1d gives a detailed breakdown of the cell parameters.

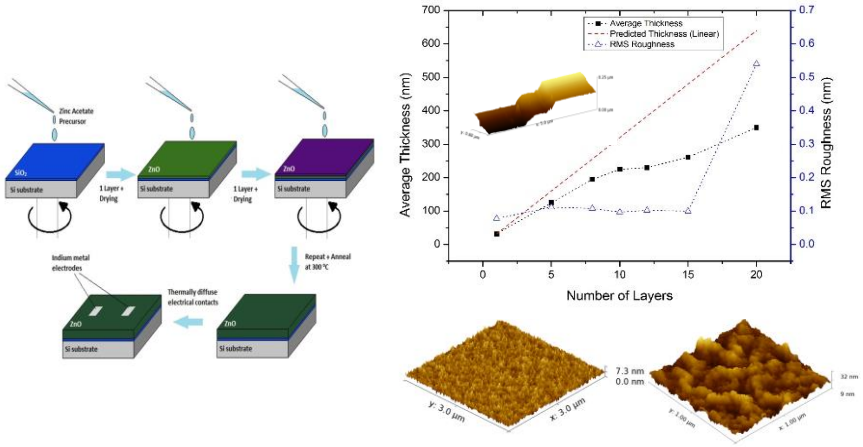
References:

1 Wang, W.; Winkler, M.T.; Gunawan, O.; Gokmen, T.; Todorov, T.K.; Zhu, Y.; and Mitzi, D.B., *Adv. Energy Mater* 2014 4 (7) ,
2 Singh, A.; Geaney, H.; Laffir, F. and Ryan, K.M., *J. Am. Chem. Soc.*, 2012, 134 (6), 2910
3 Miskin, C.K.; Yang, W.C.; Hages, C.J.; Carter, N.J; Joglekar, C.S.; Stach, E.A. and Agrawal, R, *Prog. Photovolt: Res. Appl.* 2014, 23(5), 654

Email: Gerard.bree@ul.ie

Defect Removal in Solution-Processable ZnO for Thin Film Transistors

Buckley, D.* and O'Dwyer, C.
[a] *Department of Chemistry, University College Cork, Cork T12 YN60, Ireland*



Abstract:

Solution based, thin film transistors (TFTs) are examined for their promise in next-generation, high-pixel transmission displays. High mobility metal oxides including ZnO are well suited for TFT technology on transparent substrates for see-through electronics. We show that iterative spin-coating of ZnO-based precursors can fabricate thin, transparent and uniform films on glass and channel materials on gate dielectric-coated silicon substrates. Characterisation of the crystallinity, morphology, O-vacancy formation, stoichiometry, surface roughness and thickness variation was determined through X-ray diffraction, scanning electron and atomic force microscopy, and X-ray photoelectron spectroscopy, and the data of multi-layered ZnO correlated to defect formation and electrical conductivity. Spin-coated ZnO thin films with thickness ranging between 15 - 30 nm per layer after annealing at 300 °C are found to increase overall thickness non-linearly with the number of deposited layers, suggesting a porosity infilling mechanism that iteratively erases pinhole defects. Results show that the film's surface morphology was very smooth, with average rms roughness <0.15 nm. 2-probe *I-V* measurements confirmed improved conductivity with increasing film thickness.

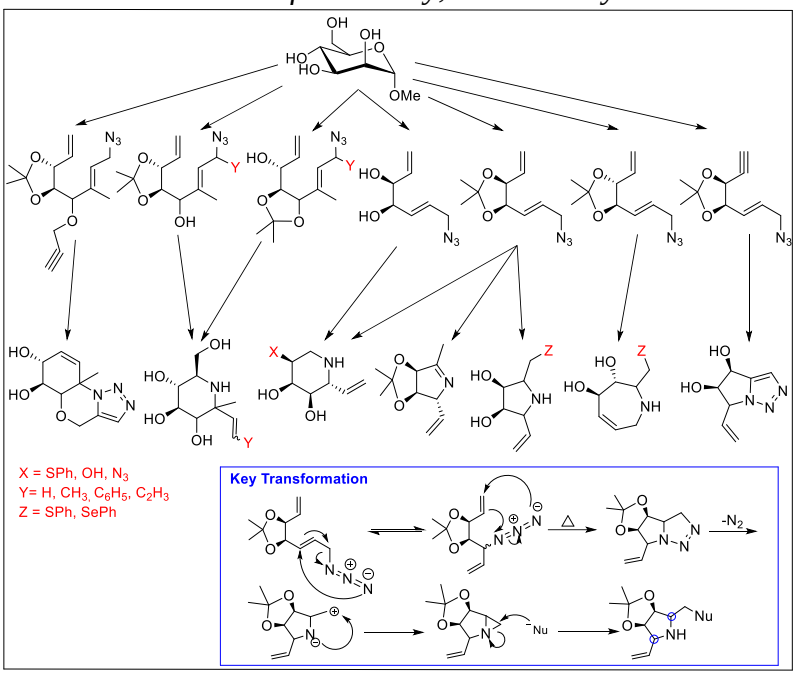
References:

1 Street, R. A. *Advanced Materials*, 2009, 21 (20), 2007.
2 Nomura, K.; Ohta, H.; Takagi, A.; Kamiya, T.; Hirano, M.; Hosono, H. *Nature* 2004,432(7016), 488.
3 Hwang, Y. H.; Jeon, J. H.; Seo, S.-J.; Bae, B.-S. *Electrochemical and Solid-State Letters* 2009, 12 (9), H336.
4 Armelao, L.; Fabrizio, M.; Gialanella, S.; Zordan, F. *Thin Solid Films* 2001, 394 (1–2), 89.

Email: darbuckley@gmail.com

The Allylic Azide Rearrangement in Tandem with Huisgen Cycloaddition: A diversity orientated synthesis to new scaffolds

Chadda, R.*; Murphy, P.V.
School of Chemistry, NUI Galway



Abstract:

Iminosugars are a class of naturally occuring polyhydroxylated alkaloids that have proven clinical applications. The high bioactivity of these sugar mimics is predominantly attributed to their inhibition of glycosidases. However, in recent years they have also shown activity as immune modulators, chaperones of misfolded proteins, peptidomimetics or new scaffolds for medicinal chemistry. As a result there has been an increased effort to synthesise libraries of these small molecules in an attempt to fine-tune this type of compound or scaffold for drug discovery. A new route has recently been developed in the Murphy group[1] at NUI Galway to access manno-, altro- and gluco- C-glycosyl iminosugars from the corresponding D-sugar. More recent work on exploring the use of this tandem reaction, in a stereoselective manner, C-glycosyl compounds in 5- ring systems and quaternary centres at the anomeric position in 6- ring systems will be presented (scheme).

References:

1 Moynihan, L.; Chadda, R.; McArdle, P.; Murphy, P.V. *Org. Lett.*, 2015, 17 (24), 6226-6229

Email: r.chadda1@nuigalway.ie

Multiphysics simulations of microbattery architectures and Cu-Ge core-shell anode nanostructure for lithium ion energy storage applications.

Clancy, T.M * and Rohan, J.F.
Tyndall National Institute
University College Cork

Abstract:

The Internet of Things is the development and integration of wireless sensors into everyday objects that allow them to send and receive data. The main issues that are associated with the wireless sensors are energy provision and storage, which means increased performance per unit substrate area are therefore required. Li-ion microbattery lifetimes are 5,000+ cycles with the use of solid state electrolytes and additive free thin film cathode materials have resulted in limitations in performance. The cathode, which is the capacity limiting electrode, thickness is restricted to micrometres and thus large surface areas are required resulting in a battery dominated by packaing.

Li-ion microbatteries are the most energy dense option but have limited areal storage capacity and power delivery capability. In this poster, multiphysics simulations (COMSOL) of the active materials in 3D, 1D and core-shell architectures have shown that nanoscale and core-shell nanowires of relatively low conductive $LiCoO_2$ can operate within the appropriate potential range (cut-off voltage 2.5 V) at almost 3 times the C-rate in comparison with micron scale thin film materials.

Germanium (Ge) anode nanostructures is an alternative to a Li metal anode, as it can potentially hold 4 times more energy density (mWh cm-2) per µm than Li metal, the most common anode in microbatteries. However, Ge suffers mechanical instability (for micron scale material) due to volume expansion and contraction on cycling. Nanostrucutures with a high electronic conductivity supports such as copper nanotubes[1] enhance mechanical stability at the nanoscale while also increasing the surface area and increasing the rate capabilities. This research builds on the fabrication process of the copper nanotubes and analysis of high energy dense materials in nanostructured architectures to evaluate the Ge anode nanostructures. [2, 3]

References:

1 Hasan, M. Chowdhury, T. and Rohan, J.F. *J. Electrochem. Soc*, 2010, 157, A682.
2 Rohan, J.F. Hasan, M. Patil, S. Casey, D. and Clancy, T. *ICT-Energy concepts towards Zero-Power Information and Communication Technology*, 2014, Chapter 6,
3 Clancy, T. Hasan , M. and Rohan, J. F. *ECS Transactions*, 2014, 61, 21.

Email: james.rohan@tyndall.ie.

Chiral Mn_3O_4 nanoparticles for enantioselective heterogeneous catalysis

Cleary, O. * and Gun'ko, Y.K.
Trinity College Dublin

Abstract:

Chiral Mn_3O_4 nanoparticles have been synthesised by a hydrothermal method and characterised by a variety of techniques including transmission electron microscopy, circular dichroism spectroscopy and x-ray powder diffraction. Nanocrystalline metal oxides demonstrate great promise as heterogeneous catalysts[1] and when modified with appropriate surface functionality, have been shown to catalyse a number of enantioselective reactions[2-5].
Chiral Mn_3O_4 nanoparticles modified with a number of different surface functionalities are currently being investigated as enantioselective heterogeneous catalysts in selected organic transformations.

References:

1. J. Hu, L. Chen and R. Richards, in *Metal Oxide Catalysis*, Wiley-VCH Verlag GmbH & Co. KGaA, Editon edn., 2009, pp. 613-663.
2. M. L. Kantam, T. Ramani, L. Chakrapani and K. V. Kumar, *Tetrahedron Letters*, 2008, **49**, 1498-1501.
3. M. L. Kantam, K. V. S. Ranganath, K. Mahendar, L. Chakrapani and B. M. Choudary, *Tetrahedron Letters*, 2007, **48**, 7646-7649.
4. M. L. Kantam, J. Yadav, S. Laha, P. Srinivas, B. Sreedhar and F. Figueras, *The Journal of Organic Chemistry*, 2009, **74**, 4608-4611.
5. C. Chen, H. Shi and G. Zhao, *The Journal of Physical Chemistry C*, 2014, **118**, 12041-12049.

Email: clearyol@tcd.ie

Development and Characterisation of Innovative Hybrid Sol-Gel Materials for the Protection of AA2024-T3

[1,2]Maikki Cullen, [1]Dr. Mohamed Oubaha, [1]Dr. Brendan Duffy
CREST, Focas Institute, Dublin Institute of Technology, Camden Row, Dublin 8
School of Chemical and Pharmaceutical Sciences, Dublin Institute of Technology, Kevin Street

Currently, corrosion protection for aluminium in the aerospace industry is provided by toxic chromate VI-based coatings, used under derogation by the industry. However, due to the high toxicity of hexavalent chromium, environmentally benign alternatives are strongly needed with no viable solutions proposed so far. Hence, there is a strong need in the development of innovative eco-friendly technologies for the replacement of chromate coatings.

The aim of this work is to develop new environmentally friendly sol-gel systems that can be used to coat both free and anodized aluminium, thereby reducing corrosion. The solution proposed here consists of employing the sol-gel process to develop fully densified hybrid organic and inorganic coatings that fulfils the required aerospace anticorrosion standards (ASTM B117). The hybrid sol-gel materials that are central to this research are liquid-phase materials compatible with most coating deposition processes, such as dip-, spin- and spray-coating. They are materials containing organic and inorganic components at a molecular level, synthesized by means of hydrolysis and condensation reactions of inexpensive alkoxide precursors. Key to the development of highly anticorrosive sol-gel coatings is the investigation of the densification process to achieve highly densified coatings. In order to do this, the strategy consists of optimising the sol-gel formulations along with the curing methodologies. Here, the development of dual interpenetrating sol-gel systems are investigated employing both organosilane and transition metal networks.

The relationship between the structure of the nanomaterials and their anticorrosion performances are investigated using a range of characterisation techniques, including PDS, NSS, SEM, FTIR and DLS. It is shown that the performances of the sol-gel coatings are dependent on the transition metal concentration and the hydrolysis degree. The leading coatings on blank AA2024-T3 panels exhibited a corrosion resistance of 168 hours in neutral salt spray. It is found that the key issue with the anticorrosion resistance is related to the adhesion of the sol-gel coating on the Aluminium substrate. Therefore, future work consists of investigating the adhesion promotion strategies to improve the corrosion resistance of our sol-gel systems.

Investigation of Iodine in relation to marine boundary fog formation in real time by use of the WIBS (Wideband Integrated Bioaerosol Sensor) and SMPS (Scanning Mobility Particle Sizer)

Author(s): Shane M. Daly[1], Eoin McGillicuddy[1], Stig Hellebust[1], David Healy[1], Jovanna Arndt[1], Paddy Feeney[1], Michael Quirke[1], David J. O'Connor[1,2], John C. Wenger[1] and John R. Sodeau[1]

Corresponding Author Institution: [1]Department of Chemistry and Environmental Research Institute, University College Cork, Cork, Ireland.
[2] School of Chemical and Pharmaceutical Sciences, Dublin Institute of Technology, Dublin, Ireland.

Abstract:

The Wideband Integrated Bioaerosol Sensor (WIBS) is the modern tool that is being increasingly deployed for on-line bioaerosol monitoring. It provides a real-time profile of airborne fluorescent and non-fluorescent particles by means of fluorescence spectroscopy and optical scatter. Biological particles (e.g. pollen, fungal spores) contain fluorophores (e.g. amino acids) that are detectable after light excitation. WIBS can also identify size and asymmetry (shape) of the particles by use of laser scattering. However, many chemical particles also weakly fluoresce. To date no strongly fluorescing airborne chemical particles have been detected by WIBS in the 0.5-22 µm size range over which the technique is operative. The WIBS-4 was deployed in Haulbowline Island for a field campaign over the following dates: 15th July to 31st July 2011 and 1st September to 30th September 2011. (Haulbowline is an island off the coast of Cork). The WIBS was accompanied by a Scanning Mobility Particle Sizer (SMPS) to provide a more in-depth analysis of the particles over a more extensive size range (10 ~ 450 nm). During the campaign multiple fog formation events occurred and coincided with escalations in the recorded fluorescent particle counts. The question arose then as to whether or not biological release events gave rise to the fogs. However, various properties of these particles are also consistent with the release of iodine-containing particles from sea-shore kelp. These releases to give rise to molecular iodine, iodine oxides and iodochlorine (ICl) are well known to occur in coastal areas from previous studies. Therefore, the spectroscopic, optical and spectrometric properties of the aerosols present were investigated to see if the results can be attributed to the release of biological particles and/or iodine-related species.

Corresponding Author Email: shane_daly@umail.ucc.ie

Novel Photoelectrochemical Fuel Cell System Utilizing Nanoparticulate Ceria Photocatalysts

Rafaela C.de Carvalho*, Anthony Betts, John Cassidy

CeO_2 nanoparticles were synthesized by a novel simple colloidal procedure. The impact of different factors like temperature and reactants concentration were varied experimentally, and optimized for CeO_2 nanoparticle synthesis. These nanoparticles were characterized by different techniques as UV-vis spectrometer, Raman, EDS, XRD, DLS and SEM to obtain information about absorption spectrum, elemental analysis, mean crystallite size, size distribution and morphology of nanoparticles. The data obtained by these analyses indicated that the colloidal method produces nanoparticles with a size range of 2-8nm.

Degradation of pollutants in wastewaters by photocatalysis is well known. In addition to this project the nanoparticles were utilized for photocatalytic degradation behavior of the dye Methyl orange in aqueous solution. CeO_2 in both colloidal and powder forms were utilized as the catalyst under an irradiance of a sun simulator, which has given successful results. By utilizing this photocatalytic process in a Photo Fuel Cell (PFC) device, their rate of destruction may be greatly enhanced, at the same time producing useful electrical energy. This novel nanocrystalline visible-light active cerium oxide (ceria) photocatalysts will be incorporated onto a range of conductive surfaces for use as photoanodes in PFCs. Their behavior in a PFC device will be assessed using selected wastewater pollutants and biomass-sourced compounds. A range of environmental conditions will be explored such as fuel/pollutant concentration level, electrolyte composition and pH variation, in order to determine the best performing catalyst/support/environment combination. A transition metal oxide-based air cathode will also be used (replacing expensive platinum) in conjunction with a modified PFC design, thus characteristics and mechanistic insights will be ascertained as a result. Direct comparison will be made with PFCs using a standard nanoparticulate TiO_2 photocatalyst.

References:

- A Garcia, R Espinosa, L Delgado, E Casals, E Gonzalez, V Puntes, C Barata, X Font, A Sanchez, *Desalination* , 269, 136 (2009)
- P Enright, PhD Thesis "*Development of Photoassisted Fuel Cell*", DIT (2009).
- P Enright, A J Betts, J F Cassidy, *Journal of Applied Electrochemistry, 41*, 345 (2011).
- S K Mudili, S Wang, S Chen, C F Ng, C H A Huan, T C Sum, H S Soo, *Beilstein Journal of Nanotechnology*, 5, 517 (2014)

Email: rafa_cdc@hotmail.com

Direct bandgap $Ge_{1-x}Sn_x$ nanowires

Doherty, J.[1], Biswas, S.[1], Saladukh, D.[3], Ramasse, Q.[4] and Holmes, J.D.[1,2]

[1]Materials Chemistry & Analysis Group, Department of Chemistry and the Tyndall National Institute, University College Cork, Cork, Ireland. [2]AMBER@CRANN, Trinity College Dublin, Dublin 2, Ireland. [3]Department of Photonics, Tyndall National Institute, University College Cork, Cork, Ireland. [4]SuperSTEM Laboratory, SciTech Daresbury Campus, Daresbury WA4 4AD, United Kingdom.

Abstract:

The development of non-equilibrium group IV nanoscale alloys is key to achieve new functionalities, such as direct bandgap, in conventional indirect bandgap elemental semiconductors. Group IV one-dimensional nanoscale systems are critical for the advancement of silicon compatible device modules. In particular, direct bandgap semiconductor materials are needed for new device architectures such as "band-to-band tunnelling (BTBT)" tunnel FETs (TFET), optical interconnects and for the development of group IV photonics. Here, we describe for the first time the fabrication of uniform diameter, direct bandgap $Ge_{1-x}Sn_x$ alloy nanowires, with a Sn incorporation up to 9.2 at.%, through a conventional catalytic bottom-up growth paradigm employing innovative catalysts and precursors. Sn inclusion in the Ge nanowires far exceeded the equilibrium solubility (~ 1 at.%) of Sn in bulk Ge. The addition of an annealing step close to the Ge-Sn eutectic temperature (230 ºC) during cool-down, facilitated the excessive dissolution of Sn in the nanowires. Sn was uniformly distributed throughout the Ge nanowire lattice, as determined by atomic resolution energy electron loss spectroscopy, with no metallic Sn segregation or precipitation at the surface or within the bulk of the nanowires. A direct bandgap has been identified for $Ge_{1-x}Sn_x$ nanowires with 9.2 at.% Sn through temperature and power dependent photoluminescence. The non-equilibrium incorporation of Sn into the Ge nanowires can be understood in terms of a kinetic trapping model for impurity incorporation at the triple-phase boundary during growth.

Email: jessica.doherty@umail.ucc.ie

REAL TIME MONITORING OF OXIDATIVE STRESS IN A MODEL OF PARKINSON'S DISEASE

Doran, M.M. *; Finnerty, N.J. and Lowry, J.P.

Department of Chemistry, Maynooth University, Maynooth, Co Kildare

Parkinson's disease (PD) produces a range of symptoms, including tremor, rigidity, slowness of movement, and problems with balance and coordination. Patients may also have memory problems, depression, and sleep complaints. Animal models have been extensively used to study neuronal and behavioural alterations caused by PD[1]. The administration of reserpine to rodents has been suggested as a pharmacological model of PD based on the effects of this monoamine-depleting agent on motor activity. Reserpine interferes with the storage of monoamines in intracellular vesicles causing monoamine depletion in nerve terminals and transient hypolocomotion and muscular rigidity depending on the dose[2]. It works by inhibiting the vesicular monoamine transporter 2 (VMAT-2). The blockage of dopamine vesicular uptake results in the accumulation of neurotoxic dopamine oxidation byproducts which potentially increases brain oxidative stress leading to neuronal damage [3]**.** In order to understand this relationship, and to determine the effects of reserpine on the sleep – wake cycle, markers of oxidative stress (e.g. NO, H_2O_2 and O_2) where monitored in real time using implanted sensors in freely-moving animals.

Supported by the Irish Research Council (Project ID RS/2012/152) and the John and Pat Hume Scholarship.

References:

(1) Beal, M. F. *Nature Reviews Neuroscience*, 2001, *2*, 325.
(2) Fernandes, V. S.; Santos, J. R.; Leão, A. H. F. F.; Medeiros, A. M.; Melo, T. G.; Izídio, G. S.; Cabral, A.; Ribeiro, R. A.; Abílio, V. C.; Ribeiro, A. M.; Silva, R. H. *Behavioural Brain Research*, 2012, *231*, 154.
(3) Caudle, W. M.; Colebrooke, R. E.; Emson, P. C.; Miller, G. W. *Trends in Neurosciences*, 2008, *31*, 303.

Email: michelle.doran@nuim.ie

Photo-responsive materials functionalised with spiropyran derivatives

Dunne, A*.; Francis, W.; MacArdle, S.; Hennessy, J.; Florea, L**. and Diamond, D.
Insight Centre for Data Analytics, NCSR, School of Chemical Sciences,
Dublin City University

Abstract:

Photo-responsive hydrogels of varying compositions containing spiropyran photochromic units have been widely studied in recent years due to their many potential applications, including photo-actuated micro-valves for microfluidic devices [1,2].

In this work two hydrogel formulations were developed producing reversible photo-responsive hydrogel actuators operative in neutral pH. Both compositions contain the photochromic unit spiropyran acrylate (SP) and acrylic acid (AA) copolymerised in the main polymer backbone, together with *N*-isopropylacrylamide (NIPAAm) or acrylamide (AAm), respectively. At neutral pH, the AA comonomer dissociates to the acrylate anion (A^-) transferring the proton to the SP unit to give the more hydrophilic protonated merocyanine ($MC\text{-}H^+$) form, which triggers water uptake and hydrogel expansion. Under white light irradiation, the $MC\text{-}H^+$ reverts to the more hydrophobic SP isomer with simultaneous reformation of acrylic acid. These simultaneous processes reduce the overall hydrophilicity of the polymeric chain through different mechanisms, triggering hydrogel contraction.

In the case of p(NIPAAm-*co*-AA-*co*-SP) hydrogel, the optimum composition has resulted in an area contraction of up to 45% of its fully hydrated size after 4 min of white light exposure, followed by reswelling to up to 85% of the initial size after 11 min in the dark.

In comparison, optimized p(AAm-*co*-AA-*co*-SP) hydrogels have resulted in contraction of ~15% in diameter within 90 seconds of white light irradiation followed by reswelling to ~95% of its fully hydrated size after ~30 seconds in the dark.

In both cases the photo-induced contraction/reswelling processes were reversible and repeatable over at least 3 cycles with no detectable hysteresis.

These hydrogels were further used for the development of improved photo-responsive valves in microfluidic devices and light guided “walkers” capable of phototactic movement.

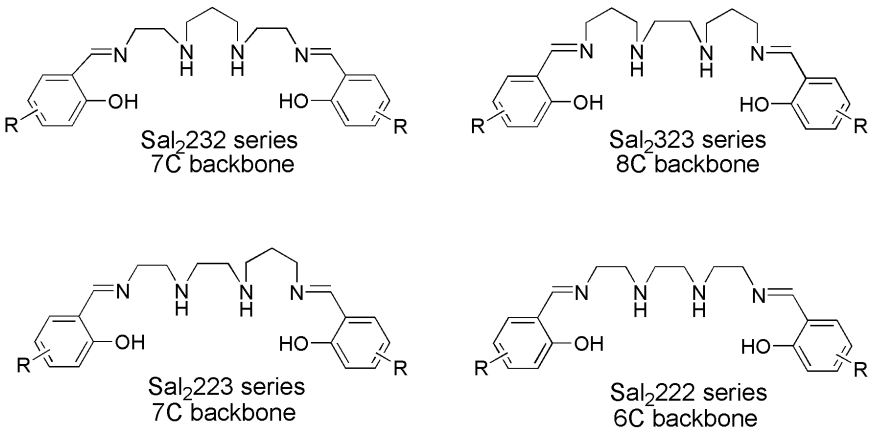
References:

[1] Ter Schiphorst, J., Coleman, S., Stumpel, J.E., Ben Azouz, A., Diamond, D., Schenning, A.P.H.J., 2015. Chem. Mater. 27, 5925–5931.
[2] Ziółkowski, B., Florea, L., Theobald, J., Benito-Lopez, F., Diamond, D., 2013. Soft Matter 9, 8754 – 8760.

Email (**): larisa.florea@dcu.ie

The role of ligand symmetry in spin-labile mononuclear Mn(III) complexes

C. Evesson,* M. M. Harris, H. Müller-Bunz, C. J. Harding, S. Shakespeare, G. G. Morgan.
School of Chemistry, University College Dublin, Belfield, Dublin 4, Ireland



Abstract:

Mononuclear Mn(III) complexes are highly prized in catalysis,[1] particularly in water oxidation[2] and increasingly in molecular magnetism.[3] In our work we have concentrated on the ability of mononuclear Mn(III) complexes to exist in both high spin (HS) and low spin (LS) forms when co-ordinated by flexible hexadentate Schiff-base ligands of the Sal_2323 series,[4] and many of these also show spin crossover.[5,6]

We are now interested in breaking the symmetry in the parent ligand and investigating the effect this has on the resulting Mn(III) complexes in terms of geometric constraint, orbital populations, magnetic properties and reactivity. We present here structural, magnetic and spectroscopic data on several Mn(III) complexes with 7 carbon backbone ligands which show a range of spin states and unusual reactivity.

References:

1 Q. Shi, Z. Shi, N. Li, Y. Tang, W. Li and H. Tang, *Curr. Org. Chem.*, 2013, **17**, 2936–2970.
2 X. Liu and F. Wang, *Coord. Chem. Rev.*, 2012, **256**, 1115–1136.
3 O. Kahn, *Annu. Rep. Prog. Chem.*, 2007, **103**, 20–38.
4 B. Gildea, M. M. Harris, L. C. Gavin, C. A. Murray, Y. Ortin, H. Müller-Bunz, C. J. Harding, Y. Lan, A. K. Powell and G. G. Morgan, *Inorg. Chem.*, 2014, **53**, 6022–33.
5 G. G. Morgan, K. D. Murnaghan, H. Müller-Bunz, V. McKee and C. J. Harding, *Angew. Chemie - Int. Ed.*, 2006, **45**, 7192–7195.
6 P. N. Martinho, B. Gildea, M. M. Harris, T. Lemma, A. D. Naik, H. Müller-Bunz, T. E. Keyes, Y. Garcia and G. G. Morgan, *Angew. Chemie - Int. Ed.*, 2012, **51**, 12597–12601.

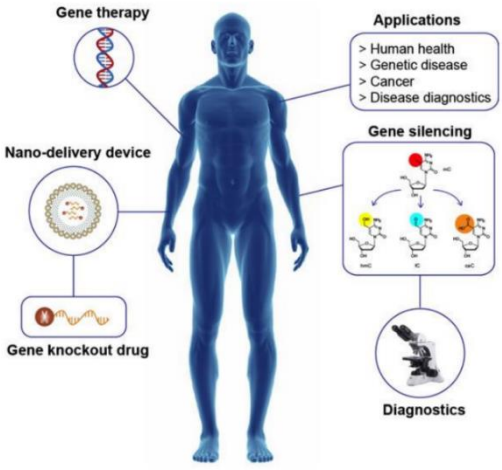
Email: colin.evesson@ucdconnect.ie.

ClickGene: Click Chemistry for Future Gene Therapies to Benefit Citizens, Researchers and Industry

Fantoni, N.[a*], Lauria, T.[a*], Avella, G.[b*], Barron, N.[b], Kellett, A.[a]
a) School of Chemical Sciences, National Institute for Cellular Biotechnology and Nano-Bioanalytical Research Facility, Dublin City University, Glasnevin, Dublin 9, Ireland.
b) School of Biotechnology and National Institute for Cellular Biotechnology, Dublin City University, Glasnevin, Dublin 9, Ireland.

Abstract:

Gene therapy is a growing field that aims to discover new molecules and therapeutics for personalised use within molecular medicine. In this context, the Marie Curie Innovative Training Network, ClickGene, is focused on the development of the next-generation gene silencing therapeutics and epigenetic DNA probes. This project focuses on artificial metallonuclease (AMN) development as these agents represent an intriguing choice of gene silencing agent given their ability to both target and oxidatively damage DNA. Sigman's reagent, $[Cu(1,10\text{-phenanthroline})_2]^{2+}$, represents the cornerstone of these AMNs, but elicits non-specific oxidation of DNA through cleavage of the C-H deoxyribose bond at the C1' position.[1a] Taking inspiration from this complex,[1b,c] a new class of compound has been designed to offer a unique mechanism for DNA cleavage compared with the current state-of-art gene editing nucleases found in zinc finger nucleases and TALENs. Furthermore, these newly developed AMNs will be tethered by "click" chemistry to sequence-selective nucleic acid targeting molecules such as zinc finger proteins and triplex forming oligonucleotides which can discriminate epigenetic bases (*e.g.* methylated and unmethylated sequences). This project aims also to create customised liposomal nanoparticle and nanocontainer delivery vehicles for highly specific delivery of these AMN bioconjugates to the nucleus of selected human cells.



This work was supported by Marie Sklodowska-Curie Innovative Training Network (ITN) ClickGene (H2020-MSCA-ITN-2014-642023). www.clickgene.eu

References:

1 (a) Fantoni, N.; Lauria, T.; Kellett, A. *Synlett.*, **2015**, *26* (19), 2623; (b) Slator, C., Barron N., Howe O., Kellett, A. *ACS Chem. Biol.*, **2016**, *11* (1), 159; (c) Larragy, R., Fitzgerald, J., Prisecaru, A., McKee, V., Leonard, P., Kellett, A. *Chem. Commun.*, **2015**, *51*, 12908.

Email: nicolo.fantoni2@mail.dcu.ie; terry.lauria90@virgilio.it; giuseppe.avella@dcu.ie;

Carbon screen-printed electrodes modified with sensing hydrogel layer for the detection of monosaccharides using electrical impedance spectroscopy

Daikuzono, C.M[1,2]*; Florea, L.[1]; Delaney, C[1]; Morrin, A.[1]; Diamond, D.[1] and Novais De Oliveira, O.[1,2]

[1]*Insight Centre for Data Analytics, National Centre for Sensor Research, Dublin City University, Dublin, Ireland*

[1]*Instituto de Fisica de São Carlos, Universidade de São Paulo, Brasil*

Here we present a novel sensor for the detection of monosaccharides (*e.g.* glucose, fructose) in solution using electrical impedance spectroscopy. The sensor is based on printed carbon interdigitated electrodes on paper using screen printing technique. The surface of the electrodes was modified with a hydrogel containing acrylamide and 20 mol% 3-(Acrylamido)phenylboronic acid (PBA). Boronic acids (BAs) are well known for their strong, reversible interactions with diol-containing compounds like sugars, such as glucose and fructose [1]. Incorporating BAs in to a hydrogel matrix can influence the volume of the hydrogel upon saccharide binding [1,2]. It was observed that the hydrogel layer containing 20 mol% PBA can swell considerably in the presence of glucose and fructose. This in turn changes the electrical conductivity of the hydrogel layer making it a suitable impedance sensor for the quantitative detection of saccharides.

We investigated the capacitance and impedance variations with different concentration of glucose and fructose (5-50 mM) present in phosphate buffer aqueous solution. The electrical measurements were made using Solartron 1260. 20 mV was applied and the impedance was analyzed in a frequency range of 0.1 – 10 MHz. The results show a decrease of impedance values with increasing sugar concentration due to less resistivity to electrical current. Aqueous solutions containing different concentrations of glucose and fructose, respectively, were then monitored through capacitance data at a frequency of 1 kHz. The results indicated that the 20 mol% PBA hydrogel swells more when in contact with fructose solution than glucose when the same concentrations of the sugar were employed. This could potentially be used to differentiate between the different sugars present in solution. Future work will focus on the incorporation of these modified carbon printed electrodes in wearable skin patch type platforms for non-invasive sugar monitoring in sweat.

References:

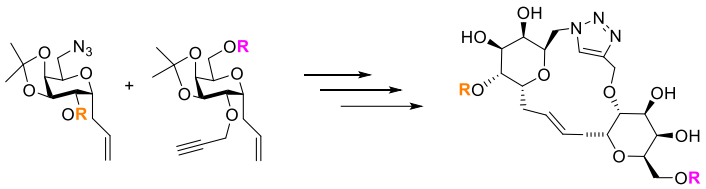
1 Zhang, C.; Losego, M.D. and Braun, P.V. *Chem. Mater*, 2013, 25, 3239-3250.
2 Guan, Y. and Zhang, Y. *Chem. Soc. Rev.*, 2013, **42**, 8106—8121

Email: larisa.florea@dcu.ie

Macrocyclic Synthesis: Potential Scaffolds for Drug Discovery

Fox, K.A* and Murphy, P.V.

NUI Galway



Abstract:

Screening in drug discovery requires structurally and functionally diverse compounds and can lead to the identification of useful modulators of biological pathways. Natural products are considered an excellent starting point when carrying out screening. However, many natural products are complex and can be difficult to isolate or synthesise. Thus synthesis of macrocyclic 'natural product like' compounds is attractive. Macrocycles serve as an important class of targets. They provide diverse functionality and stereochemical complexity. Migrastatin is an example of a macrocyclic natural product. It is a novel anti-metastatic compound of microbial origin.[1] As 90% of all cancer deaths are caused by cancer cell migration, [2] blocking this process is the main treatment strategy. Hence, the development of anti-metastasis inhibitors was explored within the Murphy group. Analogues, structurally related to migrastatin, were synthesised and evaluated, yielding promising results.[2] Additionally the synthesis of bifunctional saccharide-derived macrocyclic compounds, glycotriazolophanes, were also explored leading to the identification of an inducer of apoptosis in leukemic cells.[3] Described will be the synthesis of a diverse library of building blocks based on migrastatin and simple carbohydrates and their subsequent combination, which will lead to the formation of macrocyclic scaffolds that may be of interest as metastasis inhibitors.

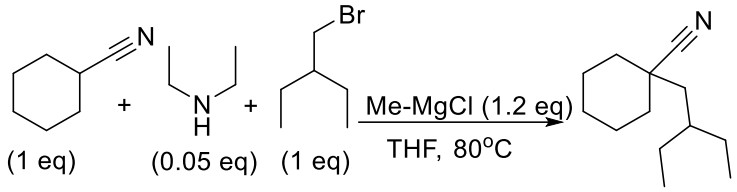
References:

1. Woo EJ, Starks CM, Carney JR, et al. Migrastatin and a new compound, isomigrastatin, from Streptomyces platensis. *J Antibiot (Tokyo)*. 2002;55(2):141-6
2. Majchrzak K, Lo Re D, Gajewska M, et al. Migrastatin Analogues Inhibit Canine Mammary Cancer Cell Migration and Invasion. *PLoS One*. 2013;8(10):1-13.
3. Zhou J, Reidy M, O'Reilly C, et al. Decorated Macrocycles via Ring-Closing Double-Reductive Amination. Identification of an Apoptosis Inducer of Leukemic Cells That at Least Partially Antagonizes a 5-HT2 Receptor. *Org Lett*. 2015;17(7):1672-1675.

Email: k.fox1@nuigalway.ie

Investigation of methylmagnesium chloride as a non-nucleophilic base

Gbadebo, O*, and O'Leary, P.
School of chemistry, National Univerisity of Ireland, Galway



Scheme: Synthetic route by Roche

Abstract:

Methyl magnesium chloride (Me-MgCl) is a key reagent industrially and in research. It is applied in a wide variety of synthetic applications (1). In 2012, the pharmaceutical company Roche patented a new process (2) in which they have been able to establish the use of Me-MgCl as a non-nucleophilic base in conjunction with catalytic amounts of an amine mediator to deprotonate alpha to a nitrile in alkylation reactions.

Grignard reagents are generally known to undergo nucleophilic additions with nitriles but, although only 5mol% of the amine mediator is used, there is virtually no attack observed at the nitrile.

This poster will describe our exploration of the use of the Me-MgCl as a non- nucleophilic base in a large number of reactions using different electrophiles and nucleophiles. Its application to key synthetic concepts such as asymmetric reactions by the use of chiral mediators such as chiral amines will also be discussed.

References:

1. Tamao K, Sumitani K, Kumada M. J. Am. Chem. Soc., 1972, **94** (12): 4374-6.
2. Harnett GJ, Hayes J, Reents R, Smith DA, Walsh A. New Process. Google Patents; 2011 (patent US 2012/0071683 A1).

Email: O.GBADEBO2@NUIGALWAY.IE.

Investigations on the mechanical forces required for mechanochemical synthesis of hydroxyapatite

Griffin, C.S.*; Kelly, C.B.; Croker, D.M and Walker, G.M.

Synthesis and Solid State Pharmaceutical Centre (SSPC),
Department of Chemical and Environmental Sciences,
Bernal Institute
University of Limerick

Abstract:

Mechanochemistry is the field of science which studies chemical reactions induced by mechanical energy[1]. This paper focuses on the synthesis of hydroxyapatite, a bone substitute biomaterial, by mechanochemical synthesis, and in particular in determining the mechanical forces required for the solid state reaction to occur.

Hydroxyapatite was synthesised from calcium hydroxide and diammonium phosphate in a Retsch Mixer Mill MM 400, varying both the milling time and milling frequency. The solid state reaction was undertaken using molar ratios of calcium hydroxide and diammonium phosphate according to the following reaction equation:

$$10Ca(OH)_2 + 6(NH_4)_2HPO_4 \rightarrow Ca_{10}(PO_4)_6(OH)_2 + 12NH_3 + 18H_2O$$

The formation of hydroxyapatite and reaction yield was analysed by powder x-ray diffraction (XRD) and Raman spectroscopy.

The impaction forces in the ball mill were estimated based on the mass and acceleration of the milling media in the mill jar, according to the following equation:

$$F = ma$$
$$m = mass\ of\ milling\ ball\ (kg);\ a = acceleration\ of\ milling\ ball\ (m/s^2)$$

The acceleration of the milling ball was calculated using the milling frequency, the dimensions of the milling jar and the pattern of the milling media inside the mill jars.

References:

1. Baláž, P. *et al.* Hallmarks of mechanochemistry: from nanoparticles to technology. *Chem. Soc. Rev.* **42,** 7571–637 (2013).

Email: Ciara.Griffin@ul.ie

Reversible Disassembly of Manganese-Based Coordination Networks

Healy, C.;* Tandon, S.; Watson, G.; Schmitt, W.
Trinity College Dublin

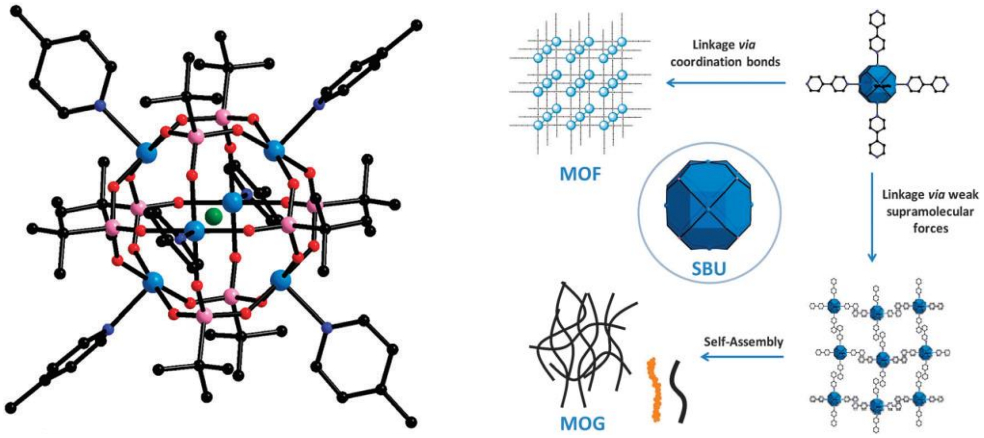


*Fig. 1: (left) The {Mn_6} core of **1** and **2**, where L=4-picoline. (right) The {Mn_6} core can be combined into networks (frameworks or gels), which in turn can be reversibly disassembled, allowing reversible capture and release of guest molecules.*

Abstract:

Coordination Networks (frameworks or gels) have long attracted attention for application as storage materials for a variety of guest molecules. However the facile release of these guests represents an ongoing challenge.[1] Here, we present network structures constructed from octahedral manganese coordination clusters $[ClMn_6(t\text{-}BuPO_3)_8(L)_6]^+$ (**1**) and $[BrMn_6(t\text{-}BuPO_3)_8(L)_6]^+$ (**2**).[2] These cationic networks can be charge-balanced by a variety of anionic guests, including halides, carboxylates, and simple metal-oxides.

Placing mild stimuli on the network structures (*e.g.* addition of competitor ligands) causes them to disassemble into their solution-phase building blocks, releasing the anionic guests into solution. Standard homogenous reactions (*e.g.* redox catalysis) may be carried out using these guests in solution. Removal of the stimulus regenerates the framework, allowing the recapture of the guests into a heterogeneous storage matrix.

References:

1 Heinke, L.; Cakici, M.; Dommaschk, M.; Grosjean, S.; Herges, R.; Brase, S.; Woll, C. *ACS Nano*, 2014, 8, 1463.
2 Zhang, L.; Marzec, B.; Clerac, R.; Chen, Y.; Zhang, H.; Schmitt, W. *Chem. Commun.*, 2013, 49, 66.

Email: healyc6@tcd.ie

Rational Design and Development of Novel Metal – Based Chemotherapeutic Agents

Kenny, R.G.* and Marmion, C.J.
The Royal College of Surgeons in Ireland

Abstract:

Platinum-based chemotherapeutics such as cisplatin are among the most commonly used treatments for cancer.[1] Despite their clinical success, they have drawbacks; they are highly toxic towards healthy cells and thus have severe dose-limiting toxic side effects. Some cancer cells also possess intrinsic or acquired resistance to these treatments. Cisplatin binds to DNA nucleobases leading to the inhibition of cellular functions and ultimately to the induction of apoptosis. Recent studies into the development of new metal-based drugs have attempted to add biologically active moieties to the cisplatin framework to create multi-functional chemotherapeutic drugs which have cellular targets beyond DNA.

Previous work in our group involved the successful development of dual functional platinum complexes with histone deacetylase (HDAC) inhibitors as ligands. These complexes demonstrated cytotoxicity comparable to cisplatin both *in vitro* and *in vivo* but with a significantly reduced level of toxicity towards healthy cells.[2] Building on this work, we have rationally designed, through molecular modelling studies, multi-functional metal drug candidates with a view to further enhancing the therapeutic efficacy of existing therapies. The rationale behind their development and results obtained to date will be presented.

References:

1 (a) Johnstone, T. C.; Suntharalingam, K.; Lippard, S. J. Chem. Rev. 2016, 116, 3436; (b) Parker, J.P.; Ude, Z.; Marmion, C.J. Metallomics, 2016, 8, 43.

2. (a) Griffith, D.; Morgan, M.P.; Marmion, C.J. *Chem. Comm.*, 2009, 44, 6735-6737; (b) Brabec V, Griffith D.M.; Kisova A.; Kostrhunova H.; Zerzankova L.; Marmion C.J.; Kasparkova J. Mol. Pharm. 2012, 9, 1990.

Email: reecekenny@rcsi.ie

CSCB Centre for Synthesis & Chemical Biology

RCSI

Bismuth Hydroxamic Acid Complexes as Potential anti-H. Pylori Agents

Donal M Keogan*, Deirdre Fitzgerald-Hughes, Darren M Griffith.
Centre for Synthesis & Chemical Biology, Department of Pharmaceutical and Medicinal Chemistry, RCSI, Dublin 2, Ireland

Abstract:

Helicobacter pylori is a microaerophilic and neutralophilic Gram negative bacterial pathogen that colonises the human stomach and is associated with gastrointestinal disorders including dyspepsia, peptic ulcers and is the strongest known risk factor associated with gastric cancer. Recently *H. Pylori* has been associated with a growing number of extragastric conditions such as iron deficiency anaemia, Parkinson's disease and heart disease. Rates of *H. Pylori* infection are currently estimated to be 20-50% in industrialised nations and up to 80% in developing countries.(1)

The continuing rise in antibiotic resistance has caused a marked decrease in the efficacy of standard first line treatments for *H. Pylori* and despite concerted effort to select suitable drugs and tailor parameters such as dosage, dosing intervals and treatment duration an effective treatment regimen for *H. pylori* has not been established yet. There is therefore an urgent need to develop novel strategies for effectively combating *H. pylori*.

Progress in relation to the development of novel bismuth hydroxamic acid complexes as potential anti-H. pylori agents will be reported as well as their activity against different strains of *H. pylori* and isolated Urease enzyme. These compounds will target *H. pylori* via two independent mechanisms; the well-known bactericidal activity of bismuth(III) ions and inhibition of urease via hydroxamic acids.

This research is supported by the Irish Research Council under Project ID GOIPG/2014/693.

References:

1 Keogan DM, Griffith DM. Molecules. 2014; 19: 15258-15297.

Email: donalkeogan@rcsi.ie

Structural studies of a series of benzene-1,3,5-tricarboxamide derivatives

Lynes, A.D.*[a]; Hawes, C.S.[a]; Ward, E.[b]; Pal, R.[b]; Gunnlaugsson, T.[a]
[a]*School of Chemistry and Trinity Biomedical Sciences Institute, Trinity College Dublin.*
[b]*Department of Chemistry Durham University South Road, Durham, DH1 3LE (UK)*

Abstract:

Benzene-1,3,5-tricarboxamide (BTA) derivatives have been widely studied in supramolecular chemistry for many years. Owing to their relatively simple synthesis and the wide range of derivatives available, they find applications in a wide range of areas, for example, nanotechnology and biomedical applications.[1] A family of eight BTA compounds, with varied side arm functionality, were synthesised, characterised and investigations into their supramolecular self-assembly behaviour were carried out. The results of these experiments revealed that the nature of the side chain had a significant impact on the type of structures formed, with long carbon chain carboxylic acid derivatives tending towards gelation, while ester derivatives displayed liquid crystal behaviour. The introduction of aromatic groups on the side chains gave rise to coordination polymers when reacted with d-block metal ions.

I (a) ences:

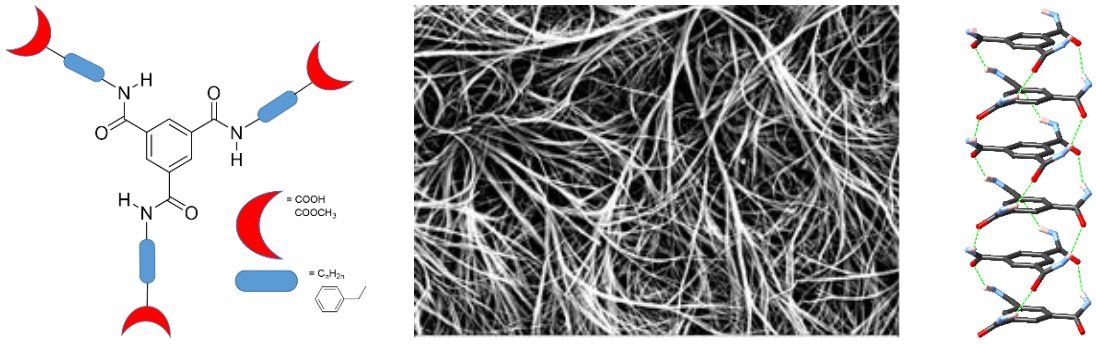


FIGURE 1 (A) GENERAL STRUCTURE OF COMPOUNDS STUDIED; (B) SEM OF THE GEL NETWORK FORMED BY THE CARBOXYLIC ACID DERIVATIVES; (C) CRYSTAL STRUCTURE OBTAINED OF ONE OF THE ESTER DERIVATIVES

1. Cantekin, S.; de Greef, T. F. A.; Palmans, A. R. A., *Chem. Soc. Rev.* **2012,** *41* (18), 6125-6137.

Email: lynesa@tcd.ie

Microfluidic Sol Gels for Medical Sensing – Microsense

MacHugh, E*; Oubhaha,M. and Duffy,B

Centre for Research in Engineering Surface Technology- CREST,
School of Chemical and Pharmaceutical Sciences, Dublin Institute of Technology, Dublin (Ireland)

Abstract:

Currently within the medical diagnostics industry the majority of diagnostic testing takes place in centralized hospital laboratories. This testing process is time consuming and uses both expensive and large scale equipment and testing must be carried out by experienced lab personnel [1]. In recent years the increase in biosensor development has led to the use of inexpensive biosensor point of care devices [1]. Currently the point of care devices available are only typically capable of testing for a single parameter. Such is the case with glucose meters which have revolutionised diabetes care. However single analyte testing is not always sufficient, particularly for early detection of diseases such as cancers and cardiovascular diseases, where parallel monitoring of multiple analytes is needed.

Therefore this project aims to address this issue by creating a novel sol gel based microfluidic optical biosensor platform, which would be capable of detecting and quantifying trace amounts of multiple biomolecules with both a high degree of sensitivity and selectivity simultaneously. A standard photolithography fabrication process will be used to microstructure the photo curable hybrid organic/inorganic sol gel material. Optimisation of the photocurable sol gel material will be carried out using both chemical and physical methods. The curing time and photoreactiviy of the optimised sol will also be investigated. This optimisation will then be used for rapid soft photolithographic processing of the microfluidic biosensor, in particular focusing on the relationship between photoreactivitity, structure of the material and the optical properties of the material. Suitable photo- iniators will be selected to maximise the photoreactivity of the sol gel material. Novel sensor coatings with an integrated microfluidic system will be used as a fabrication process. At the end of the project a point of care device that is compatible for industry and commercialisation is expected to be developed.

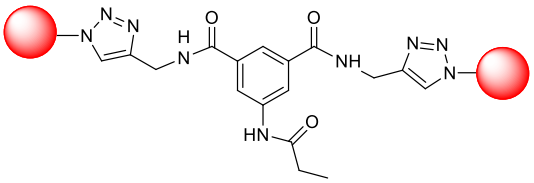
References:

1. Yeo,L.Y.;Chang,H.C.;Chan,P.P.Y.;Friend,J.R.; *Small*,2011,7,12.

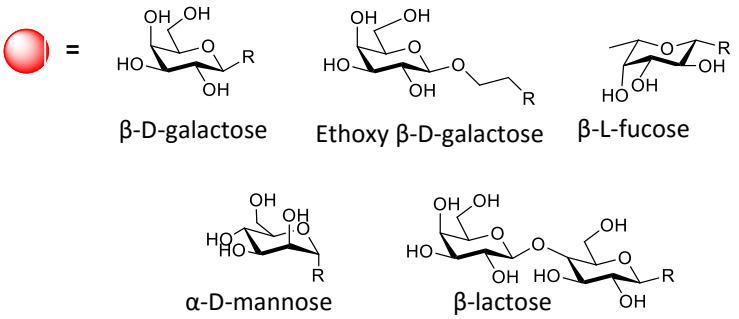
Email: emma.machugh@mydit.ie

Glycoconjugates To Prevent Candida Albicans Adhesion

Martin, H.*; Velasco-Torrijos, T. and Kavangh, K.
Maynooth University



Divalent ligand



Abstract:

Anti-adhesion therapy can be used to prevent infectious diseases caused by fungi and bacteria. Anti-adhesion ligands interfere with the ability of the fungi or bacteria to adhere to cells in the host organism.[1, 2] This form of therapy is needed since the inappropriate use of antibiotics has led to an increase in fungal and bacterial strains resistant to this form of treatment.

In this study, anti-adhesion compounds of *Candida albicans* in buccal epithelial cells (BEC) are considered. It was found that glycomimetics built around aromatic scaffolds could be potential immunomodulators. Using synthetic carbohydrate chemistry and Copper-Catalyzed Azide-Alkyne Cycloaddition (CuAAC) chemistry[3], monovalent, divalent and trivalent anti-adhesion ligands were synthesised. It was found that the divalent galactose ligands showed the best anti-adhesive properties. The aim of this project is to fluorescently label the ligands to investigate the inhibition of *C. albicans* adhesion to the BEC surface produced by the glycoconjugate ligands.

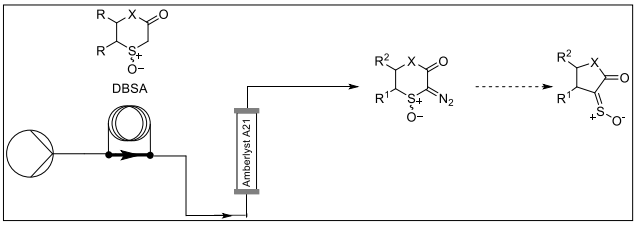
References:

1 Bavington, C. *Respiration*, 2005, 72, 335.
2 Sharon, N. *Biochimica et Biophysica Acta (BBA) – General Subjects*, 2006, 1760, 527.
3 Presolski, S.I.; Hong, V.P. and Finn, M.G. *Current Protocols in Chemical Biology*, 2011, 3, 153.

Email: harlei.martin.2012@mumail.ie

Synthesis and reactivity of α-Diazosulfoxides in a continuous flow system

McCaw, P.G.*, Maguire, A.R. and Collins, S.G.
Department of Chemistry and ABCRF, University College Cork, Ireland.
Cork, Ireland.



Abstract:

In 1968, Hodson and Holt described α-diazosulfoxides as an unstable moiety.[1] Subsequent work by our group successfully synthesised for the first time a series of stable, isolable bicyclic and monocyclic α-diazo-β-oxo-sulfoxides in good yields, by diazo transfer to the corresponding sulfinyl lactones and lactams.[2]

In related work by our research group, the reactivity of these α-diazosulfoxides has been investigated. Using transition metal catalysis, microwave irradiation, photolysis or thermolysis, dediazotisation of the α-diazosulfoxide leads to an α-oxo carbene,[3-5] which then undergoes a hetero-Wolff rearrangement to an α-oxo sulfine intermediate. This very useful reactive sulfine intermediate can follow a number of different reaction pathways including cycloadditions or nucleophilic additions.[6]

All previous work on α-diazosulfoxides in the group had been done in batch reactions, herein we report initial exciting results on transferring the process to a continuous flow system. Utilisation of dodecylbenzenesulfonyl azide over the traditionally used reagent tosyl azide provides the reaction with an improved safety profile. Limiting the exposure of the products to basic conditions by careful control of the residence time, led to a 2-3 fold increase in yields and a significant reduction in reaction time. The substrate scope has been expanded to include lactone and ketone derived sulfoxides and subsequent generation and trapping of the reactive α-oxo sulfine in the continuous flow reactor formed stable novel heterocycles.

References:

(1) Hodson, D.; Holt, G. *J. Chem. Soc. C: Org.* **1968**, 1602.
(2) Collins, S. G.; O'Sullivan, O. C. M.; Kelleher, P. G.; Maguire, A. R. *Org. Bio. Chem.* **2013**, *11*, 1706.
(3) Maguire, A. R.; Kelleher, P. G.; Lawrence, S. E. *Tetrahedron Lett.* **1998**, *39*, 3849.
(4) O'Sullivan, O.; Collins, S.; Maguire, A. *Synlett* **2008**, *2008*, 659.
(5) Sander, W.; Strehl, A.; Maguire, A. R.; Collins, S. G.; Kelleher, P. G. *Eur. J. Org. Chem.* **2000**, *2000*, 3329.
(6) McCaw, P. G.; Buckley, N. M.; Collins, S. G.; Maguire, A. R. *Eur. J. Org. Chem.* **2016**, *2016*, 1630.

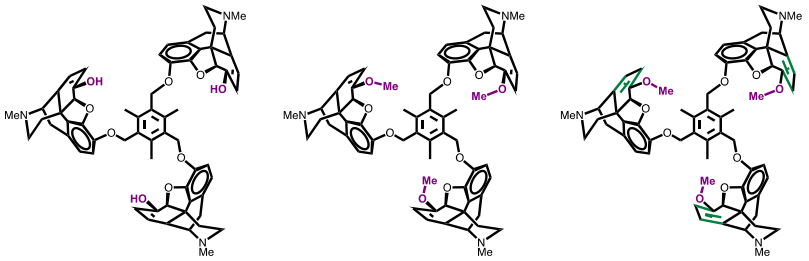
OPIOID ARCHITECTURES AS NEW DNA BINDING MOLECULES

McStay, N.[1*]; Molphy, Z.[1*]; Cafolla, T.[2]; Coughlan, A.[1]; Gathergood, N.[3]; and Kellett, A[1].

[1]School of Chemical Sciences, National Institute for Cellular Biotechnology, and Nano-Bioanalytical Research Facility, Dublin City University, Glasnevin, Dublin 9, Ireland. [2]School of Physical Sciences Dublin City University, Glasnevin, Dublin 9, Ireland. [3]Chair of Green Chemistry, Department of Chemistry, Tallinn University of Technology, Akadeemia tee 15, 12618 Tallinn, Estonia.

ABSTRACT:

The discovery of new synthetic DNA recognition agents is an area of considerable research interest. The quest to discover new materials that non-covalently interact with DNA carries tremendous application to the areas of human health and biomedical diagnostics. Non-covalent DNA binding agents have already found widespread utility as antitumoural agents[1] as probes for the fluorescent labeling and detection of nucleic acids[2] and as condensation agents[3] that efficiently package nucleic acids for gene delivery (transfection) to mammalian cells. Herein we report the synthesis of tripodal C_3-symmetric opioid scaffolds as efficient condensation agents of duplex DNA (dsDNA). Condensation was achieved on both superhelical and linear dsDNA conformations and identified by agarose electrophoresis, viscosity, turbidity, and atomic force microscopy (AFM) measurements. Structurally, we identify the requirement of a C_3 scaffold for condensation as both di- (C_2-symmetric) and mono-substituted (C_1-symmetric) opioid-functionalised mesitylene derivatives were effectively unable to coordinate dsDNA. Condensation, identified by both toroidal and globule AFM aggregation, arises from surface-driven ionic bonding between the protonated, cationic, tertiary amine group on the opioid skeleton and the phosphate nucleic acid backbone. Indeed, by masking the phenolic hydroxy group of morphine (**MC3**) with methoxy substituents in heterocodeine (**HC3**) and oripavine (**OC3**), dsDNA compaction is retained thus negating phosphate—hydroxyl surface-driven interactions. This presents a summary of our recent findings on the DNA binding properties of new C_3 symmetric opioid structures. These architectures are first to our knowledge where the opioid class has demonstrated effective DNA binding affinity and may now open up a new frontier for semi-synthetic frontier for nucleic acid drug research.



REFERENCES:

1 Marks, P. A. and Breslow, R. *Nat. Biotechnol.*, **2007**, 25**,** 84-90.

2 Spink, N., Brown, D. G., Skelly, J. V., and Neidle, S. *NAR*, **1994**, 22**,** 1607-1612.

3 Malina, J., Farrell, N. P., and Brabec, V. *Angew. Chem. Int. Ed*, **2014**, 53**,** 12812-12816. Prisecaru, A.; Molphy, Z.; Kipping, R. G.; Peterson, E. J.; Qu, Y.; Kellett, A.; Farrell, N. P. Nucleic Acids Res. **2014**, 42 (22), 13474–13487.

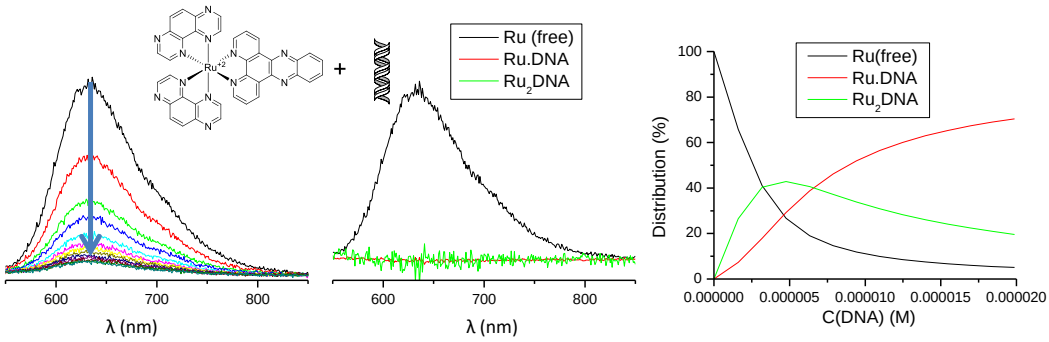
Email: natasha.mcstay2@mail.dcu.ie

Spectroscopic study of DNA-ligand binding with multi-wavelength data

Poulsen, B.C.,* Estalayo, S.A., Blaco, S., Bright, S., Poynton, F.E., Kelly, J.M., Williams, D.C., Gunnlaugsson, T.
School of Chemistry, Trinity Biomedical Science Institute, Trinity College Dublin

Abstract:

Ruthenium polypyridyl complexes with derivatives of dipyrido[3,2-a:2',3'-c]phenazine (**dppz**) as one of the ligands have shown to be promising in biological application as DNA binding ligands.[1] This includes potential as luminescent dyes for imaging or photodynamic therapeutic agents in cancer therapy. In this work has been studied the binding to DNA of a series of complexes with **dppz** or its derivatives as ligands together with 1,10-phenanthroline (**phen**) or 1,4,5,8-tetraazaphenanthrene (**TAP**) as ancillary ligands. The binding to DNA has been studied with different techniques including absorption and emission spectroscopy, circular (CD) and linear dichroism (LD), and viscometry. The binding affinity and stoichiometry have been calculated from the change in the absorption and emission spectrum at increasing concentration of DNA by the use of non-linear regression analysis of multi-wavelength absorption and emission data. All complexes were found to bind strongly to DNA with binding constants in the order of 10^6 M^{-1}. The spectral changes for the complexes upon binding to DNA, including the changes in the CD and LD spectra, indicate intercalation that is confirmed by a large increase in the viscosity in accordance with a lengthening and stiffening of the DNA helix.



References:

1 Cloonan, S.M.; Elmes, R.B.P.; Bright, S.A.; Erby, M.L.; Poynton, F.E.; Nolan, D.E.; Quinn, S.J.; Gunnlaugsson, T. and Williams, D.C. *J. Med. Chem.*, 2015, 58, 4494.

Email: Gunnlaut@tcd.ie

Sound Bending Chemical Reactions: Non-Titrimetric Determination of Acid-Base Reactions using BARDS.

M. Rizwan Ahmed and Dara Fitzpatrick

Abstract

Is it possible to determine an acid-base reaction without a pH probe, indicator and titres of reagent from a burette?! Is it also possible to follow the same reaction with nothing more than a microphone or even by ear? We present data which demonstrates for the first time how acid-carbonate reactions can be monitored accurately by acoustic measurements.

The stoichiometric reactions yield specific quantities of carbon dioxide which cause reproducible changes to the compressibility of the reaction mixture. This in turn slows down the speed of sound in solution which is generated by allowing the reaction vessel to resonate, which is induced by the magnetic follower inside.

Broadband Acoustic Resonance Dissolution Spectroscopy (BARDS) harnesses this phenomenon for several applications.[1] However, in this study, acid (HCl) and base (Carbonate) were reacted in stoichiometric equilibrium, to record a BARDS time –frequency acoustic spectra. The BARDS spectra obtained depend on the limiting reagent. Therefore an excess of one over the other will not produce a greater quantity of carbon dioxide. For this reason, one addition of a reagent in excess is enough to determine the end point without the need for titrimetry.

BARDS analysis also demonstrated a similar behaviour for reaction between HCl and carbonates irrespective of their counter ions (Na and K). The data also shows how half the amount of a diprotic acid is required to neutralise the same amount of carbonate as HCl to yield the same spectra for both. This is also irrespective of the counter ion of the carbonate. This method can be used to interrogate the acidity of any reaction solution in a rapid manner and may be important in situations where it is crucial that the acid is spent in a reaction mixture.

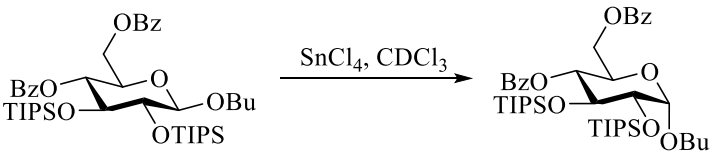
References

[1] Fitzpatrick, D., Krüse, J., Vos, B., Foley, O., Gleeson, D., O'Gorman, E., O'Keefe, R., 2012. Principles and applications of broadband acoustic resonance dissolution spectroscopy (BARDS): A sound approach for the analysis of compounds. Anal. Chem. 84, 2202–2210.

Email: 111220368@umail.ucc.ie

Synthesis of silylated sugars, studies on their anomerisation

Roux, A.* and Murphy, P.V.
National University of Ireland, Galway

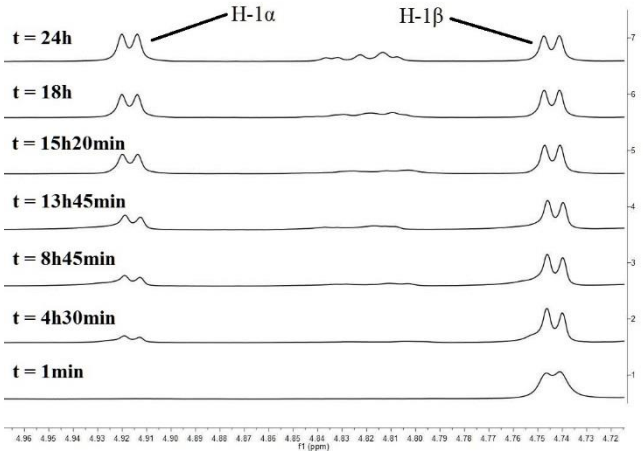


Scheme 1 Anomerisation of a silylated sugar, study of its rate of anomerisation

Abstract:

The anomerisation reaction is a reaction that is well known in carbohydrate chemistry (epimerisation of anomers). It has potential in stereoselective glycoside synthesis, with potential to give agents that could be used for treating a variety of conditions.

In our research group[1], we aim to study factors which influence the kinetics of the reaction. One approach is to vary the protecting group of the saccharide. In glycosidation it is known that silyl protecting groups can lead to more rapid reactions[2] and therefore we wish to study if this is the case for anomerisation also. In order to do that, several compounds containing different silyl based protecting groups at different hydroxyl groups on a glucopyranose have been synthesized, and their different rate of anomerisation are determined and then compared between each other. Results on the kinetics of anomerisation of these silyl derivatives will be presented on the poster.



References:

1 Pilgrim, W.; Murphy, P. V. J. Org. Chem. 2010, 75, 6747.
2 Hsu, Y.; Lu, X. A.; Zulueta, M. M.; Tsai, C. M.; Lin, K. I.; Hung, S. C.; Wong, C. H. J. Am. Chem. Soc. 2012, 134, 4549.

Email: a.roux1@nuigalway.ie

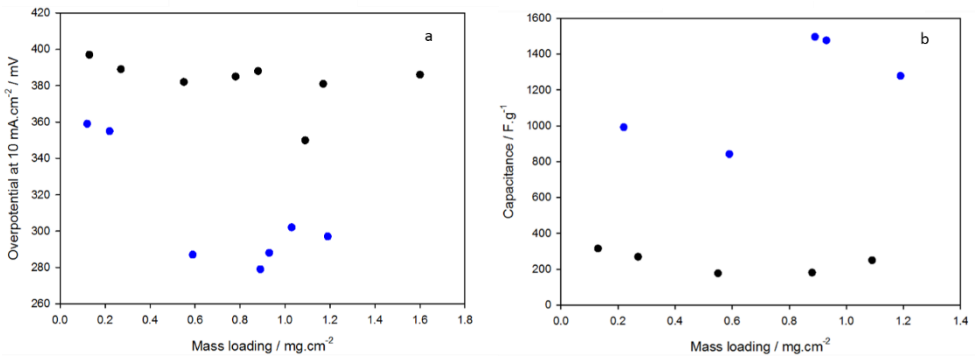
Cobalt Oxide Nanoflakes Electrodes for Supercapacitor and Oxygen Evolution Application

Rovetta*, A.A.S.; Browne, M.P.; Harvey, A.; Coleman, J.N.; Lyons, M.E.G.
Trinity College Dublin

Abstract:

Transition metal oxides have shown promising behaviour as catalysts and supercapacitors[1]. Liquid exfoliation[2] of bulk metal oxides has been recently shown to provide ready access to 2-dimensional nanoflakes, the size of which can be readily varied, with potential use in the areas of energy storage and conversion.

The production of hydrogen from the electrolysis of water is not energetically efficient because of the high anodic overpotential associated with the oxygen evolution reaction (OER). The latter is a kinetically demanding and inefficient step compared with the hydrogen evolution reaction (HER) itself. Currently anodes used in industrial electrolysers which exhibit low oxygen over-potentials are based on platinum group metal oxide materials such as RuO_2 and IrO_2. However because of materials scarcity issues and high cost, their use is limited. In the present study we examine the redox behaviour and catalytic activity for OER of exfoliated nanostructured cobalt oxide $Co(OH)_2$, in aqueous base. During this study we have noted that the oxide material performance metrics such as the oxygen overpotential at 10 $mA.cm^{-2}$ and the redox capacitance are dependant on the support and mass used (figs.1).



Figs.1. (a) Overpotential values at 10 $mA.cm^{-2}$ and (b) Capacitance values for $Co(OH)_2$ films on glassy carbon (in black) and nickel foam (in blue)

References:

1 R.L. Doyle, I. Godwin, M.P. Brandon and M. Lyons, Phys. Chem. Chem. Phys 2013, 15, 13737.
2 V. Nicolosi, M. Chhowalla, M.G. Kanatzidis, M.S. Strano, J.N. Coleman, Science 2013, 340, 6139.

Email: rovettaa@tcd.ie

Development of an Integrated Sensing System for PAT Application in the Food and Beverage Industry

Scanlon, S.[1*], Hobbs, Elizabeth [2], Morris, Virginia [2] and Moore, E.J.[1]
[1] *Tyndall National Institute and the Department of Chemistry, UCC, Cork*
[2] *PepsiCo International, Little Island, Cork*

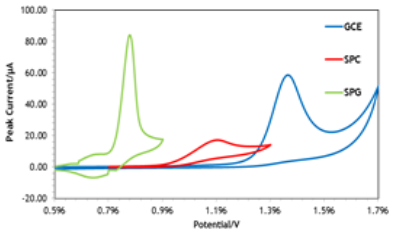


Figure 1: Cyclic voltammograms recorded at Nafion-modified glassy carbon (blue), screen printed carbon (red) and screen printed gold (green) electrodes in 0.1 M Phosphoric Acid containing 300 uM caffeine.

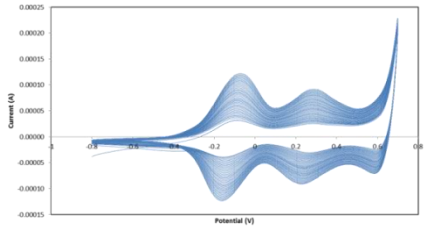


Figure 2: Cyclic voltammograms for the growth of an Iridium Oxide pH film by potentiostatic cycling in an Iridium complex solution.

Abstract:

Food and beverage quality and safety have become of significant importance over the past decade and assuring the highest standards of process control is a key priority. The FDA's Process Analytical Technology (PAT) initiative emphasises that "quality cannot be tested into products; it should be built in or should be by design" [1].

This research proposes a new system for quality control in the food and beverage industry, through the development of a multi-parameter sensing device for PAT application. Following the miniaturization of various analytical techniques, used for quality control analysis, integration into a single device will create a multi-parameter sensing system for real-time process parameter analysis. To date, much of the research has been focused on the caffeine determination, which is currently carried out off-line, using High Performance Liquid Chromatography (HPLC), which can be time consuming, with expensive instrumentation. In this work, chemical sensors for the electrochemical determination of caffeine in real samples have been developed. Three electrodes were compared, using a Nafion® modification to increase electrode sensitivity. Figure 1 shows the comparison of the three modified electrodes for the detection of caffeine, with the gold electrode proving the most efficient, even without prior pre-treatment. A low cost, re-useable sensor for the determination of caffeine in soft drink concentrate has been developed using a Nafion®-modified screen printed gold electrode. This is the first time that a sensor of its kind is used for such a purpose, with a high degree of recoverability. Work has begun on an electrochemical pH sensor, using iridium oxide modified electrodes, grown by potentiostatic cycling in an iridium complex solution, as shown in figure 2. This is the first time that an iridium oxide-modified screen printed electrode has been developed for pH determination.

References:

1 Guidance for Industry PAT-A Framework for Innovative Pharmaceutical Development, Manufacturing and Quality Assurance, United States Food and Drug Administration (FDA), September 2004

Email: shauna.scanlon@tyndall.ie

A Flexible Interpenetrated pcu Coordination Network Formed by Mixed Ligands

Mohana Shivanna*, Qingyuan Yang and Michael J. Zaworotko
Department of Chemical & Environmental Sciences, Materials and Surface Science Institute, University of Limerick, Limerick, Republic of Ireland.

Abstract:

Metal–organic materials (MOMs), also known as porous coordination polymers (PCPs) or metal-organic frameworks (MOFs), are receiving attention thanks to their amenability to design and properties [1, 3]. The pore size and chemistry of MOMs makes them excellent candidates for applications in storage, separation, sensing, and catalysis [2]. Flexible MOMs can exhibit behavior such as swelling, stepwise uptake, gate-opening and breathing which can be induced by stimuli such as solvent, pressure, heat and light [4, 5]

Here, we report a two, three-fold interpenetrated **pcu** network with general formula [Zn4(L1)4(L2)2]·DMF (L1=1,4-bis(4-carboxyphenyl)benzene;L2=1,4-bis(4-pyridyl)benzene), or L2=3,6-Di(4-pyridinyl)-1,2,4,5-tetrazine) based on axially coordinated zinc "paddle-wheels", that exhibits dynamic structural transformations induced by guest incorporation and removal. X-ray structures highlight the highly flexible nature of the framework and reveal that phase transformations involve the movement or rotation of the biphenylene dicarboxylate ligands. The coordination geometry of a zinc paddle-wheel unit is considerably changed without bond breakage.

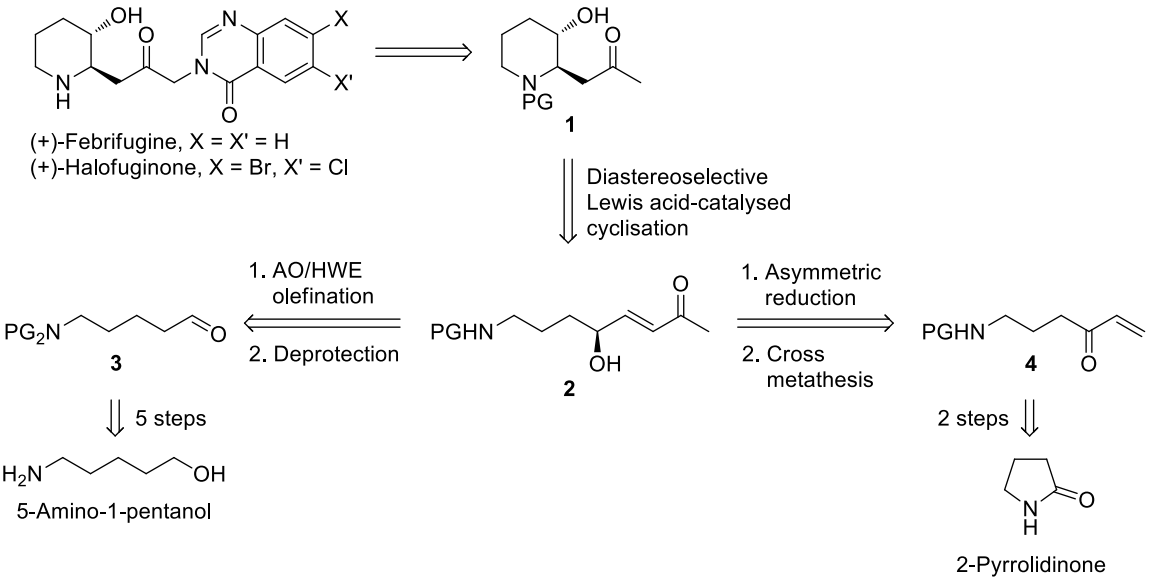
References:

1 Kitagawa, S. *et al., Chem. Soc. Rev.* **2005**, *34*, 109
2 Nugent, P. *et al., Nature*. **2013**, *495*, 80
3 Sakata, Y. *et al., science* . **2013,** *339*, 193
4 Schneemann, A. *et al., Chem. Soc. Rev*. **2014**, *43*, 6062
5 Mason, A. J. *et al., Nature*. **2015**, *527*, 357

Email: *Michael.Zaworotko@ul.ie*

Towards the Stereoselective Synthesis of Febrifugine and Analogues

Smullen, S.* and Evans, P.
Centre for Synthesis and Chemical Biology, School of Chemistry, University College Dublin, Belfield, Dublin 4, Ireland



Febrifugine,[1] an alkaloid with anti-malarial properties first isolated in the 1940s, has been the target of several synthetic routes since the 1950s. Despite febrifugine never resulting in a human treatment for malaria, it inspired the development of halofuginone for its use as an anti-protozoal agent in poultry feed (Stenerol®). During investigations into optimal dosages, halofuginone was found to possess anti-fibrotic properties and is currently in clinical trials for the treatment of Duchenne muscular dystrophy as a racemate.

The aim of this project was to develop a new stereoselective route to access both enantiomers of febrifugine and halofuginone focusing on the key piperidine-based intermediate **1**, obtained from diastereoselective Lewis acid-catalysed cyclisation of the acyclic γ-hydroxy α,β-unsaturated ketone **2**. Two routes have been developed to date: The first utilises a proline-mediated α-aminooxylation (AO)/Horner-Wadsworth-Emmons (HWE) olefination one-pot reaction of aldehyde **3** (5 steps from 5-amino-1-pentanol). The second route incorporates an asymmetric reduction of the terminal α,β-unsaturated ketone **4** (2 steps from 2-pyrrolidinone) followed by cross metathesis with methyl vinyl ketone to furnish **2**.

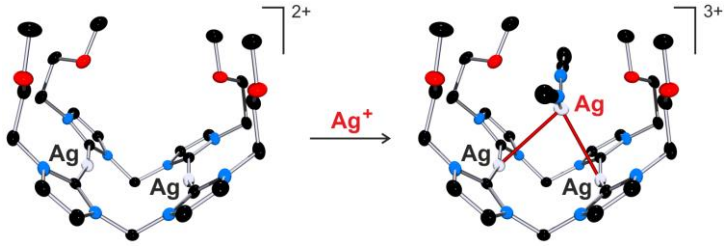
References:

1 Review, see: McLaughlin, N. P.; Evans, P.; Pines, M. *Bioorg. Med. Chem.* **2014**, *22*, 1993.

Email: shaun.smullen@ucdconnect.ie

Enhanced Metal···Metal Interactions in Cation-Cation Host−Guest Systems: {$M^+ \subset [M_2(bisNHC)_2]^{2+}$} (M = Ag, Au; NHC = N-Heterocyclic Carbene)

Vellé, A.;* Montagner, D. and Sanz Miguel, P. J.
Department of Inorganic Chemistry, University of Zaragoza, 50009 Zaragoza, Spain
Department of Chemistry, Maynooth University, Maynooth, Co. Kildare, Ireland



Abstract:

Metallophilic contacts are keystone in numerous assemblies, including in host-guest systems, nanoparticles, and in conducting, luminescent, and framework materials. Traditionally, short metal-metal distances have been characterized in the solid-state by X-ray crystallographic studies. In solution, they have been probed by spectroscopic methods (IR, Raman, UV/Vis, NMR, ESR spectroscopies). Besides, computational techniques have also been important in the study of such contacts.[1]

Recently, we observed unsupported argentophilic interactions in solution and in the solid state for a dynamic cationic silver complex, namely {$Ag^+ \subset [Ag_2(bisNHC)_2]^{2+}$} (NHC = N-Heterocyclic Carbene), which has the ability to act as an excellent host for silver ions and to aggregate in solution.[2] The unexpected strength of these metal-metal systems has been detected and studied for the first time by SAXS (small angle X-ray scattering) techniques at the molecular level.[3] We postulated that if strong donor (NHC) ligands are involved, M···M interactions involving closed-shell metal ions may be greater in length than the limits set by the van der Waals radii.[3]

We have continued our efforts to expand our investigations to more complicated systems, incorporating additional metals and bonding situations. The most important results will be presented.

References:

1 Pyykkö, P. *Chem. Rev.*, 1997, 97, 597.
2 Vellé, A.; Cebollada, A.; Iglesias, M. and Sanz Miguel, P. J. *Inorg. Chem.*, 2014, 53, 10654.
3 Cebollada, A.; Vellé, A.; Iglesias, M.; Fullmer, L. B.; Goberna-Ferrón, S.; Nyman, M. and Sanz Miguel, P. J. *Angew. Chem. Int. Ed.*, 2015, 54, 12762.

Email: avelle@unizar.es

Friday, June 24th

Session 1

BOOLE 3 & 4

Parallel Sessions

(Talks)

9.30 – 10.45 am

Applications of Fluorescent Biosensors for Non-Invasive Glucose Monitoring

Bruen, D.*; Delaney, C.; Florea, L**. and Diamond, D.
Insight Centre for Data Analytics, National Centre for Sensor Research, School of Chemical Sciences, Dublin City University, Ireland.

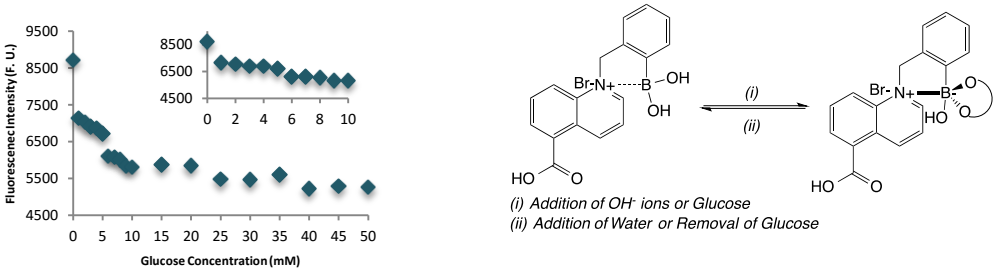


Figure 1: Direct glucose sensing using a fluorescent boronic acid derivative.

Abstract:

Diabetes is a widespread disease, whereby the body is incapable of regulating the metabolism of glucose[1]. As a result, this disorder leads to severe health effects such as blindness, kidney failure and stroke[1-2], where monitoring glucose has proven to prevent some of these undesired side effects. Current monitoring methods for diabetes are either invasive or non-continuous, where Brooks et al have introduced contact lenses, on the cover of ACS Nanomaterials, as a sensing platform for noninvasive monitoring[1]. This highlights the need for a non-invasive, continuous glucose-monitoring device for personal use[1].

Lewis acidic boronic acids (BAs) are widely known for their strong but reversible interactions with diol-containing compounds like glucose[1]. This phenomenon has lead to the development and evolution of many fluorescent boronic acid derivatives, where the BA-sugar interaction can be monitored by changes in fluorescence[1]. In our group, a range of boronic acid derivatives have been developed and investigated for their direct or indirect glucose sensing capabilities, at physiological pH. When the BA moiety is directly attached to a fluorescent component, the fluorescence of these BA-derivatives becomes quenched in the presence of glucose (**Figure 1**). The second type of fluorescence change is observed upon integration of the BA moiety and fluorophore in to a two-component system. In these sensors the introduction of the BA results in a decrease of fluorescence, which can be restored in the presence of glucose[2]. This project aims to incorporate BA derivatives on to flexible polymeric substrates for continuous non-invasive glucose sensing in wearable devices, such as sensing patches or smart contact lenses.

References:

1 Brooks, W. L. A. and Sumerlin, B. S. *Chem. Reviews*, 2016, 116, 1375-1397.
2 Yao, H.; Shum, A.J.; Cowan, M; Lanhdesmaki, I and Parviz, B.A. *Biosensors and Bioelecrtronics*, 2011, 26, 3290-3296.

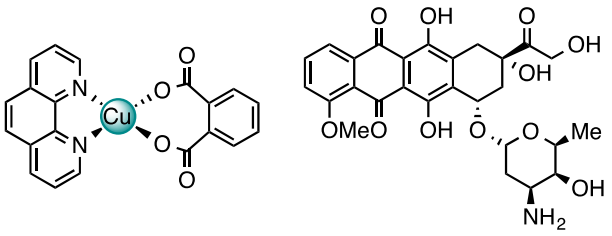
**Email: ****larisa.florea@dcu.ie

[Cu(*o*-phthalate)(phenanthroline)] Exhibits Unique Superoxide-Mediated NCI-60 Chemotherapeutic Action through Genomic DNA Damage and Mitochondrial Dysfunction

Creina Slator*, Niall Barron, Orla Howe, and Andrew Kellett
School of Chemical Sciences and National Institute for Cellular Biotechnology, Dublin City University.

Abstract:

The *in cellulo* catalytic production of reactive oxygen species (ROS) by copper(II) and iron(II) complexes is now recognized as a major mechanistic model in the design of effective cytotoxins of human cancer. The developmental copper complex ([Cu(*o*-phthalate)(1,10-phenanthroline)] (**Cu-Ph**)) is a candidate antitumoral agent that features bis-chelate—dicarboxylate and N,N′-intercalative—square planar coordination scaffold, and was reported as an intracellular ROS-active cytotoxic agent that induces double strand breaks (DSBs) in the genome of human cancer cells.[1] The cytotoxic profile of **Cu-Ph** demonstrated broad-spectrum anticancer activity within the National Cancer Institute's (NCI) Developmental Therapeutics Program (DTP), 60 human cancer cell line screen and revealed a novel mode of action to existing metal-based therapeutics via the COMPARE algorithm.[2] An extensive range of molecular methods—flow cytometry, confocal microscopy, and fluorescence spectroscopy—were applied to probe the mechanistic activity and redox targetting properties of **Cu-Ph** in intrinsically cisplatin resistance ovarian human cancer cell line, SKOV3; the studies of which were directly compared to the clinical DNA intercalator and topoisomerase II poison, doxorubicin. Employment of ROS-specific scavengers identified prevailing species, the generation of which in the are critical towards *in vitro* and intracellular mode of cytotoxic action and activation of induced cell death.



[Cu(ph)(phen)] (**Cu-Ph**) Doxorubicin (**Doxo**)

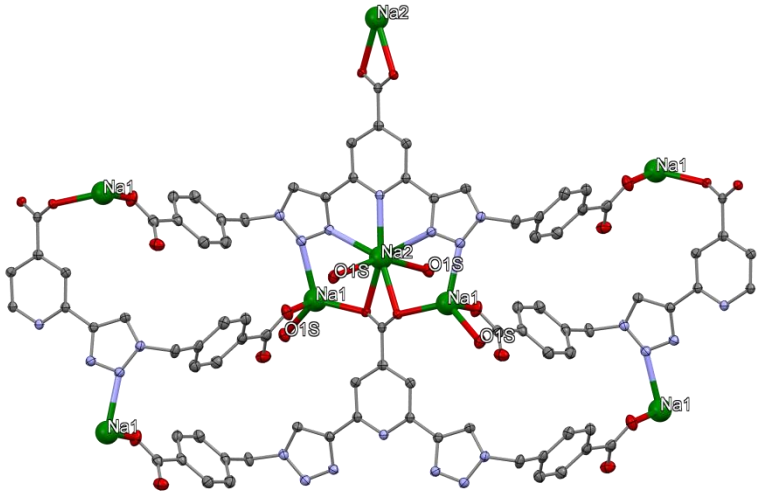
References:

1 Kellett, A., Howe, O., O'Connor, M., McCann, M., Creaven, B. S., McClean, S., Foltyn-Arfa Kia, A., Casey, A., and Devereux, M. *Free Radic. Biol. Med.*, 2012 *53*, 564.
2 Slator, C. Barron, N., Howe, O., Kellett A. *ACS Chem. Biol.*, 2016, 11 (1), 159.

Email: creina.slator2@mail.dcu.ie

Synthesis of functional supramolecular architectures the development of healable luminescent metallogels from triazole- based heterocyclic ligands

McCarney, E. P.,* Hawes, C.S., Byrne, J. P., Kitchen, J. A. and Gunnlaugsson T.
Trinity Biomedical Sciences Institute and School of Chemistry, Trinity College, Dublin,



Abstract:

Nitrogen containing heterocycles, such as triazoles, are ideal for template-directed generation of discrete polynuclear assemblies,[1] coordination polymers and novel functional nanomaterials such as gels[2] and various other intriguing architectures. Utilising host-guest chemistry in the design of diverse functional structures using appropriate organic ligands by changing metal centres has always been a keen aim in the field. We have combined the 'guest' ability of *d*- and *f*- block metal ions[3] with various versatile triazole derivative 'hosts' in the investigation of the self-assembly behaviour, and the design of healable luminescent soft matter.[4]

References:

1 W. K. C. Lo, G. S. Huff, J. R. Cubanski, A. D. W. Kennedy, C. J. McAdam, D. A. McMorran, K. C. Gordon and J. D. Crowley, *Inorg. Chem.*, 2015, **54**, 1572.
2 R. M. Meudtner and S. Hecht, *Macromol. Rapid Commun.*, 2008, **29**, 347
3 J. P. Byrne, J. A. Kitchen, J. E. O'Brien, R. D. Peacock and T. Gunnlaugsson, *Inorg. Chem.*, 2015, **54**, 1426.
4 E. P. McCarney, J. P. Byrne, B. Twamley, M. Martinez-Calvo, G. Ryan, M. E. Mobius and T. Gunnlaugsson, *Chem. Commun.*, 2015, **51**, 14123.

Email: mccarnee@tcd.ie.

Preparation and Characterisation of Supported Gold Nanoparticles with Tunable Loading and Various Applications

Belhout, S.A.[1]*; Hinds, D.T.[1]; Owen, N.[2]; Kim,J-Y.[1]; Coulter, J.[2] and Quinn, S.J.[1]
[1]*School of Chemistry, University College Dublin, Belfield, Dublin 4*
[2]*School of Pharmacy, Queens University Belfast, Belfast, BT9 7BL*

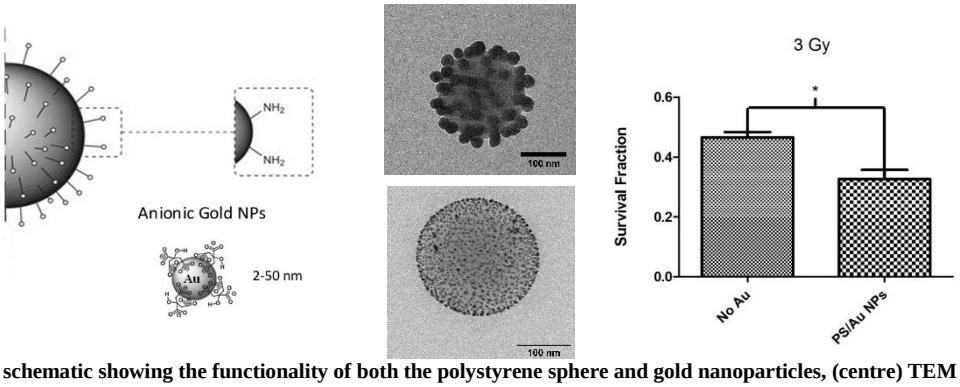


Figure 3 (left) schematic showing the functionality of both the polystyrene sphere and gold nanoparticles, (centre) TEM images showing (top) 26 nm gold nanoparticles on a 200 nm support and (bottom) 4.5 nm gold nanoparticles on a 200 nm support and (right) initial radiosensitization results showing a dose enhancement factor of 1.46

Abstract:

Tailored nanoparticle properties have wide ranging potential in areas of energy conversion, catalysis, diagnostics, sensing, imaging and therapeutics.[1] Hybrid materials comprising supported nanoparticles are advantageous as they are easy to handle and manipulate, and also provide a highly localized concentration of nanoparticles.[2] An eloquent example of their application is the use of supported particles as radiosensitizers in cells.[3,4] For diagnostic and therapeutic applications the support offers additional avenues for targeted delivery in vivo. Though a variety of methodologies exist to prepare robust composites using gels, polymer networks, micelles, microspheres, achieving controlled coating remains a key challenge. In this study the preparation of a variety of composites will be presented together with the methodologies used to quantify the gold loading, as well as the application of these hybrid materials as catalysis agents and as radiosensitizers with good dose enhancement factors when exposed to radiation. A variety of families were studied, consisting of polystyrene sphere supports (60 nm - 2000 nm) with various sized gold nanoparticles (4.5 nm - 26 nm) immobilized.

References:

[1] Eustis, S.; el-Sayed, M. A. *Chem. Soc. Rev.* 2006, 35, 209.
[2] Campelo, J. M.; Luna, D.; Luque, R.; Marinas, J.M.; Romero A. A. *ChemSusChem* 2009, 2, 18.
[3] Butterworth, K. T.; McMahon, S. J.; Currell, F. J.; Prise K. M. *Nanoscale*, 2012, 4, 4830.
[4] Jain, S. *et al. Radiother Oncol.*, 2014, 110, 342.

Email: Samir.belhout@ucdconnect.ie

Keynote Speaker

&

Closing Remarks

A Sound Approach to Analytical Chemistry

Fitzpatrick, D., Vos, B., Evans-Hurson, R., McSweeney, S., Ahmed, R., Alfarsi, A., Keating, J.J., Krüse, J.

University College Cork

Abstract:

BARDS (Broadband Acoustic Resonance Dissolution Spectroscopy) is a new platform technology which harnesses an acoustic phenomenon associated with dissolution to open up new understandings of dissolution and allows careful measurements to be made in a host of applications in the Food and Pharmaceutical sectors.[1]

The compressibility of a solution changes in a reproducible way during dissolution which can be monitored acoustically. The change in compressibility is brought about by a reduction in the solubility of gas in solution resulting in outgassing of nano- and micro-bubbles. Tablets, powder blends and custom formulations all produce an intrinsic frequency / time response during dissolution which act as a signature for the sample.

BARDS data will be presented demonstrating applications such as discrimination of polymorphs, blend uniformity, counterfeit identification, stability testing, hydration of milk proteins, non-titrimetric determination of acid-base reactions.

Dissolution can no longer be viewed as a somewhat random and chaotic process, but instead a highly ordered process in terms of changes in compressibility, outgassing and saturation yielding unique information about the solute.

References:

1 *D. Fitzpatrick, D., Krüse, J., Vos, B., Foley, O., Gleeson, D., O'Gorman, E., and O'Keefe, R., Principles and applications of broadband acoustic resonance spectroscopy, Analytical Chemistry, 2012, 84, 2202–2210.*

2 *Fitzpatrick, D., Evans-Hurson, R., Fu, Y., Burke, T., Vos, B., Krüse, J., McSweeney, S., Casaubieilh, P., & Keating, J. J. (2014). Rapid Profiling of Enteric Coated Drug Delivery Spheres via Broadband Acoustic Resonance Dissolution Spectroscopy (BARDS). Analyst, 139, 1000-1106*

Email: d.fitzpatrick@ucc.ie

ATTENDEES

Attendee	Institution
Abogunrin, Anthony	Maynooth
Aghazadeh Meshgi, Mohammad	UCC
Ahmed, Muhib	Maynooth
Ahmed, Rizwan	UCC
Alessio Verni, Giuseppe	UCC
Alfarsi, Anas	UCC
Almalki, Sameerah	UCC
Almotairy, Awatif	NUIG
Antonik, Pawel	NUIG
Ao, Xiang	Maynooth
Arribas Bueno, Raquel	UL
Banasiak, Anna	DIT
Barker, Andrew	UCD
Belhout, S.A.	UCD
Bhogala, Bala Krishna Reddy Dr	UCC
Biswas, Subhajit Dr	UCC
Bree, Gerard	UL
Brouder, Thomas	UCC
Browne, Michelle	TCD
Bruen, Danielle	DCU
Buckley, Aoife	UCC
Buckley, Darragh	UCC
Buckley, Paul	UCC
Buk, Vuslat	Tyndall
Buzid, Alayah	UCC
Cacheux, Valerie	UCC
Cano, Rafael	UCC
Cao, Xi	UCC
Carey, Trevor Dr	UCC
Carroll, Elaine	UCC
Cassidy, John Prof	DIT
Chaddha, Rekha	NUIG
Cheung, Shane	RCSI
Clancy, Tomás	Tyndall
Cleary, Olan	TCD
Colleran, John Dr	DIT
Collins, Gillian Dr	UCC
Collins, Stuart Dr	UCC
Connon, Robert	UCD

Conway-Kenny, Robert	TCD
Corina McCrellis	QUB
Creaven, Bernie	ITT
Creedon, Niamh	Tyndall
Crowley, Daniel	UCC
Cullen, Maikki	DIT
d'Agostino, Bruno	TCD
Daikuzono, Cristiane	DCU
Dalton, Hannah	TCD
Daly, Shane	UCC
Davitt, Foinan	UCC
de Carvalho, Rafaela	DIT
Deeney, Clara Dr	UCD
Doherty, Jessica	UCC
Doran, Michelle	Maynooth
Doyle, Shona	Tyndall
Driver, Ross	Maynooth
Duffy, Gerard	UCC
Dunne, Aisling	DCU
Estalayo Adrián, Sandra	TCD
Evans, Paul	UCD
Evesson, Colin	UCD
Fantoni, Nicolo	DCU
Felemban, Shifa	UCC
Fitzgerald, Desmond	UCC
Fitzgerald, Michelle	UCC
Flynn, Aaran	UCC
Foley, Aoife	UCC
Foley, Vera	UCC
Ford, Rochelle	UCD
Fox, Karen	NUIG
Franklin, Margaret	ICI
Furey, Ambrose	CIT
Gandhi, Hirenkumar	UCC
Gavin, Declan	UCC
Gaynor, Brian	UCD
Gbadebo, Lola	NUIG
Geaney, Hugh	UCC
Geraghty Niall	NUIG
Ghion, Alessandra	DIT
Gilchrist, Elizabeth	UCC
Gillen, Dermot	TCD
Glynn, Colm	UCC

Green, David	TCD
Gregory Gibson	QUB
Griffin, Ciara	UL
Griffith, Darren	RCSI
Halpin, Jennifer	Tyndall
Hargaden, Grainne Dr	DIT
Harrington, Francis	UCC
Hayden, Jack	Maynooth
Hayes, Phyllis	UCC
Healy, Colm	TCD
Heffernan, Maria	UL
Hegarty, Isabel	TCD
Helen, Lisa	UCC
Hogan, Anna	UCC
Holmes, Justin Prof.	UCC
Hourihane, Rosamund Dr	CIT
Irwin, Bryan	TCD
James, Jinju	UCD
Jones, Roisin	UCC
Judge, Eric	UCD
Kazadojev, Igor	Tyndall
Keene, Tony Dr	UCD
Kegel, Jan	Tyndall
Kelleher, Fintan Dr	ITT
Kenny, Reece	RCSI
Keogan, Donal	RCSI
Khanadavilli, Uday	UCC
Kissane, Marie, Dr	Eli Lilly
Kitteringham, Eolann	RCSI
Kruschel, Ryan	UCC
Kumar, Pavan Vydyula	UCC
Kyne, Michelle	NUIG
Langsi, Victor	UCC
Larkin, Eugene	TCD
Lawrence, Simon	UCC
Leddy, Bernard Dr	Leddy Consultant
Lehane, Mary Dr	CIT
Liu, Pai	UL
Lopez, Marystela	UL
Lu, Yue	TCD
Lynch, Denis	UCC
Lynch, Mark	UCC
Lynes, Amy	TCD

Lyons, Prof. Mike	TCD
Mac Hugh, Emma	DIT
Mackey, Katrina	UCC
Mackey, Pamela	UCC
Magtaan, Jordan	ITT
Maguire, Anita Prof	UCC
Mahon, Aine	UCD
Manley, Harry	Tyndall
Martin, Harlei	Maynooth
McCarney, Eoin	TCD
McCarthy, Laura	UCC
McCarthy, Melissa	Tyndall
McCaw Patrick,	UCC
McCormack, Declan Prof.	DIT
McKee, Mary	UCC
McKeon, Aoife	RCSI
McNulty, David	UCC
McSharry, Una	ITT
McStay, Natasha	DCU
Molina, Andres	UCC
Molphy, Zara	DCU
Moore, Eric Dr	UCC
Morelle, Luc	UCC
Mulahmetovic, Ensar	DIT
Mullin, Craig	DIT
Mullins, Nicholas Dr	DIT
Murphy, Chloe	UCC
Murphy, Noel	UCC
Murphy, Vanessa Dr	DIT
Nacca, Francesca Giulia	UCD
Newman, Gemma	ITT
NiDhubhghaill, Orla Dr	UCC
Nixon, Mathew	Maynooth
Noonan, Adrian	UCC
O'Callaghan, Katie	DIT
O'Connell, John	UCC
O'Connor, Christine Dr	DIT
O'Connor, David Dr	DIT
O'Dwyer, Colm Dr	UCC
O'Hanlon, Sally	UCC
O'Mahony, Rosella	UCC
O'Muimhneacháin, Eoin	UCC
O'Shea Kevin	UCC

O'Sullivan, Justine	Maynooth
Paranthaman, Mukesh	UCC
Pardo, Leticia	UCC
Pemble, Martyn Prof	UCC
Petkov, Nikolay Dr	CIT
Pettenuzo, Andrea	NUIG
Poulsen, Bjorn	TCD
Prabhava S.N. Barimar	TCD
Prendergast, Aisling	UCC
Quinn, Susan Dr	UCD
Ramos, Jessica	Maynooth
Reddy, Andrew	Maynooth
Reid, Caroline	Maynooth
Risse, Wilhelm Dr	UCD
Roche, Brendan	UCD
Roux, Amelie	NUIG
Rovetta, Aurelie	TCD
Ryan, Catherine	UCC
Ryan, Louise	Tyndall
Sanchez, Goar Dr	UCD
Sanyal, Nitheen Kaperi	TCD
Sarangapani, Chaitanya	DIT
Savysachi, A.J.	TCD
Scanlon, Micheal Dr	UCC
Scanlon, Shauna	UCC
Shanahan, Rachel	UCC
Shiely, Amy	UCC
Shivanna, Mohana	UL
Slator, Creina	DCU
Smith, Raymond	UCD
Smullen, Shaun	UCD
Stephens, John	Maynooth
Sullivan, David	UCC
Torrijos, Trinidad	Maynooth
Torsney Samuel	TCD
Travers, Wayne	ITT
Van Druenen, Maart	UCC
Vazquez, Patricia	UCC
Velle, Alba	Maynooth
Wang, Junsi	TCD
Wang, Yineng	UCC
Wenger, John Prof	UCC
Wilson, Eoin	UCC

Wojciechowski, Bart	DIT
Zhang, Shi Yuan	UL

NOTES