



## School News January 2023

### Welcome to....

The McGarrigle group welcomes Oana Popa, who started her PhD in January. Her PhD research focuses on stereoselective synthesis of oligosaccharides.

The Negahdar group welcomes Freya Martin, who also started her PhD in January. Freya graduated from the Chemistry with Environmental and Sustainable Chemistry program here in UCD. Her PhD research focuses on the application of dynamic catalysis for sustainable utilization of CO<sub>2</sub>.

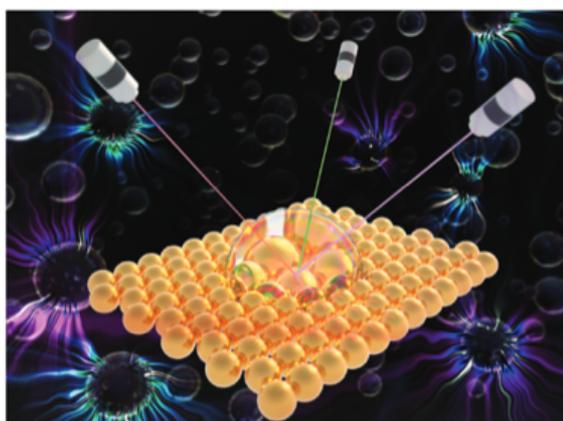
The Byrne group welcomes Thomas Rabbitte who started his PhD in January. His PhD research focuses on a mechanically-linked platform for antimicrobial agents: pairing bioactive metal complexes with lectin-targeting glycoconjugates.

A very warm welcome four new members of academic staff who recently joined the School: Assistant Professors Leila Negahdar, Aniello Palma, Joseph Byrne and Nadia Elghobashi-Meinhardt. Below you will find a brief overview of their career pathways and a glimpse at their respective research areas.



*From left-right: Assistant Professors Leila Negahdar, Aniello Palma, Joseph Byrne and Nadia Elghobashi-Meinhardt.*

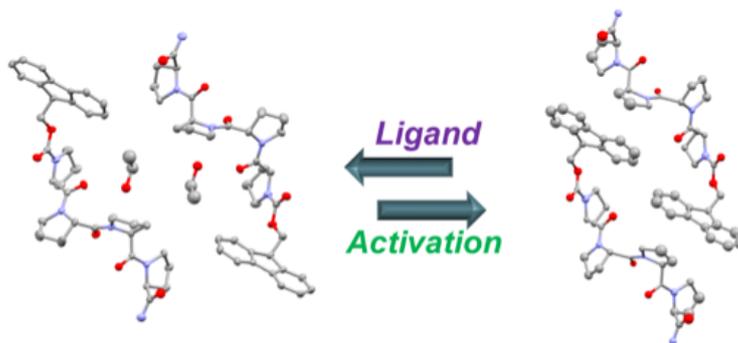
**Assistant Professor Leila Negahdar:** Before her appointment in UCD School of Chemistry, Leila was Marie Skłodowska-Curie Individual Fellow in University College London. Prior to this, she was research associate at Cardiff University UK, postdoctoral research fellow at RWTH Aachen University Germany, and postdoctoral research fellow at Utrecht University Netherlands. She received her master's degree from University of Dortmund, Germany, and PhD degree in Chemistry from RWTH Aachen University in 2015. Her research interests include mainly catalytic surface reaction, kinetics and mechanism, chemical processes and in situ/operando spectroscopy in catalysis. Her current research focuses on applying dynamic catalysis and innovative approaches for tackling the grand global challenges - climate change, pollution, and sustainable energy.



*Research highlight: Shining light on the solid–liquid interface: in situ/operando monitoring of surface catalysis*

**Assistant Professor Aniello Palma:** Aniello obtained a Master's degree in Chemistry at the Università di Napoli Federico II in 2005. In October 2010, he obtained his PhD in Organic Chemistry from UCD with a thesis entitled “Synthesis and Application of New Infra-Red Fluorophores”. In January 2011, he joined the group of Prof Anthony Barrett (FRS, FMEDSCI) in Imperial College London, as a postdoctoral researcher working on a medicinal chemistry project involving the synthesis of cyclin-dependent kinase inhibitors. In January 2015, he joined Prof Oren Scherman's research group in the Melville Laboratory for Polymer Synthesis at the University of Cambridge focusing on the synthesis of supramolecular polymers, supramolecular sensors and on the development of supramolecular catalysts. In August

2017, Aniello started his independent career in the School of Physical Sciences at the University of Kent as a Lecturer in Organic Chemistry. He joined the UCD School of Chemistry as Assistant Professor in Organic and Medicinal Chemistry in January 2023. Aniello's research focuses on the design of smart and responsive materials prepared via supramolecular approaches and inspired by biomolecules. These bioinspired materials have applications in the fields of green catalysis, chemical sensing and separation, drug delivery and novel therapeutics.

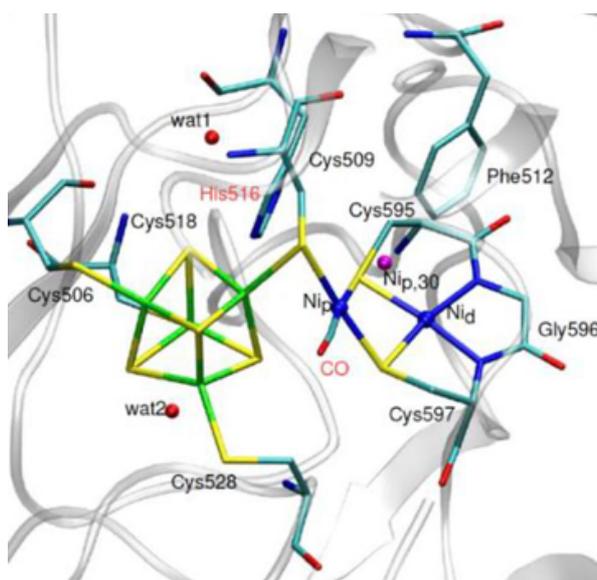


Example of a reversibly porous, crystalline, supramolecular peptide framework (SPF) developed in Palma's group. Thermal activation, guest-induced dynamic porosity and enantioselective guest inclusion have been demonstrated for this novel system. *Chem.Eur. J.* DOI: 10.1002/chem.202202368

**Assistant Professor Joe Byrne:** Joe studied chemistry first at Maynooth University and then in Trinity College Dublin where he completed his PhD in the lab of Thorri Gunnlagusson, supported by the Irish Research Council. His research was in the field of supramolecular chemistry and luminescent lanthanide complexes. He won a Marie Curie Individual Fellowship to carry out research into carbohydrate-functionalised organometallic catalysts in Martin Albrecht's group at Universität Bern (Switzerland), where he stayed for 3 years. In 2019, Joe began his independent research at University of Galway, funded by an SFI Starting Investigator Research Grant. His group have been investigating the ability of carbohydrate functionalised metal complexes to detect bacterial lectin proteins, as well as their potential antimicrobial properties. Joe joined UCD School of Chemistry in January 2023 and is leading an IRC Laureate Award and a North-South Research Project (supported by the HEA and the Shared Island Fund). New diagnostic and therapeutic tools are needed in the fight against antimicrobial resistance, and through research at the interface of inorganic chemistry and carbohydrate chemistry, the Byrne Group aim to make discoveries which will contribute to this challenge. Joe is a committee member of the RSC Carbohydrate Interest Group and the Irish Biological Inorganic Chemistry Society and advisor to the Institute of Chemistry of Ireland's Young Chemists Network.

**Assistant Professor Nadia Elghobashi-Meinhardt:** Nadia completed her PhD in Theoretical Chemistry in 2005 at the Free University Berlin, followed by two postdoctoral appointments (Fritz-Haber-Institute of the Max-Planck-Society in Berlin and Heidelberg University) to pursue research in the field of computational biophysics. In her research, Nadia uses a combination of computational techniques to study structure- function relationships in

complex biological systems. Nadia also enjoys teaching and has taught a wide range of courses in chemistry and mathematics. In 2023, Nadia was awarded a UCD Ad Astra fellowship and appointed Assistant Professor in UCD School of Chemistry.



- *Nadia's group uses quantum mechanical/molecular mechanical*
- *(QM/MM) methods to model and investigate the chemistry taking*
- *place in metalloenzymes. Here, the catalytic site of acetyl-Co-enzyme*
- *A synthase (ACS) contains an iron-sulfur cluster*

## Remembering Former Colleagues

We were saddened to learn of the recent death of Dr Ken Glass (Jan 2023), who was a Senior Lecturer in Chemistry who officially retired in 2002, after almost 40 years in UCD. Many will fondly remember him as very actively retired colleague who was on campus several days a week right up to March 2020 when the COVID-19 pandemic started. Ken played a central role in the setting up of the Chemical Services Unit, whereby the UCD Department of Chemistry provided much needed analytical services to the Irish chemical industry, and he was the director of the NMR Centre for many years having worked tirelessly at securing funds to establish it. Ken's colleagues and friends recall him as an accomplished musician, a superb chemist, an excellent supervisor, a wise advisor and a gentleman.

We were also saddened to learn of the recent death of Anthony (Tony) Brophy (Jan 2023) who was a Laboratory Attendant in Chemistry. Tony's colleagues and friends recall him as a loyal, kind, conscientious and dedicated colleague who was a great help to all those who worked with him and the students he supported.

We send our condolences to their families.

## School Events

On January 23<sup>rd</sup>, the School held a coffee morning to welcome all the new staff who have recently joined the School and to mark the start of the Spring Trimester of 2022/23.

**New staff who recently joined the School:** Leila Negahdar (Oct 2022), Aniello Palma (Jan 2023), Nadia Elghobashi-Meinhardt (Jan 2023), Joseph Byrne (Jan 2023), Kristy Stanley (Aug 2022), Michelle Doran (Aug 2022), Julia Bruno (Aug 2022), Elaine Mackey (Nov 2022).



## Awards and Recognition

Congratulations to Senior Technical Officer, Hans Eckhardt on receiving an Award for Exceptional Contribution to Learning. The award recognises individual UCD employees who are engaged directly in teaching and or facilitating student learning. Well done Hans! James Sullivan has been invited to join the editorial board of 'Sustainable Chemistry for the Environment' - an Elsevier gold open access journal.

Congratulations to Dr Robert Johnson, our resident electrochemist, who has been awarded Tenure, following an Induction period of 3 years at UCD.

Well done to the chemistry tag rugby team (pictured below), who won the Winter league plate trophy on January 11<sup>th</sup>. They are still open for sign-ups, so email [david.mc-laughlin@ucdconnect.ie](mailto:david.mc-laughlin@ucdconnect.ie) if you're interested.



### **Grant and Funding Success**

Recent grant success: Second Research Enablement Grant from the RSC to Marcus Baumann for developing flow methods for enantioconvergent reactions via new research collaboration with a team at the University of Edinburgh.

Congratulations to Gita Singh (Tony Keene's group), who received a short-term research award from E-COST-GRANT-CA19118 for the Short Term Scientific Mission (STSM) COST Action: "A step towards SUsustainable carbon as electrodes in ENER (SUS-ENERGY)". The research will be performed at Karlsruhe Institute of Technology, Germany, in March 2023.

### **New Doctor in the House**

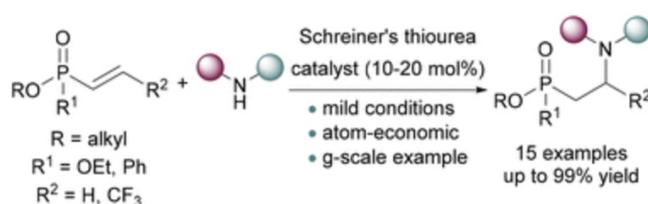
Congratulations to Dr Dennis Bengtsson from the Oscarson group on passing his viva in December.

### **Recent Publications from the School**

Congratulations to Dr George Papoutsidakis, a recent PhD graduate from Professor Vitaly Buckin's group, who published his first paper in Elsevier's Food Hydrocolloids. The work shows the capability of high-resolution ultrasonic spectroscopy to monitor the enzymatic hydrolysis of  $\beta$ -glucan by  $\beta$ -glucanase in aqueous solutions in a real-time and in a non-destructive way. The technique provided time profiles of the glycosidic bonds

hydrolyzed, the degree of hydrolysis, the number-average degree of polymerization, and molar mass. The ultrasonic results are correlated with experimental data from HPLC, viscosity, density, and reducing sugar assays. The correlation resulted in the calculation of kinetic and structural variables for the polysaccharide and its hydrolysates. Georgios I. Papoutsidakis & Vitaly Buckin, 'Real-time monitoring of enzymatic hydrolysis of 1,3(4)- $\beta$ -glucan with high-resolution ultrasonic spectroscopy', *Food Hydrocolloids*, **2023**, *138*, [108426](https://doi.org/10.1016/j.foodhyd.2022.108426).

Congratulations to Peter McDermott on his first paper from his SFI-funded PhD, describing the use of thiourea catalysis to synthesise beta-aminophosphonates.: *Org Biomol Chem* **2023**, advance article. P E McDermott, M P Ó Fearraigh, A M Horan, E M McGarrigle\*—Thiourea-catalysed conjugate additions of amines to vinyl phosphonates and phosphinates. DOI: [10.1039/D2OB02116A](https://doi.org/10.1039/D2OB02116A).



Well done to Maria Molnar, an Erasmus student from the Baumann group, who published her first paper showing an azide-free approach towards triazoles exploiting carbohydrates in flow. Maria Molnar & Marcus Baumann, 'Continuous flow synthesis of phenyl glucosazone and its conversion to 2H-1,2,3-Triazole building blocks', **2023**, <https://doi.org/10.1016/j.foodhyd.2022.108426>.

Congratulations to former Taught MSc student Adam Burke, who had his research project (summer 2022) on continuous photo-click reactions published in SynOpen. Burke A, Spiccio S, Di Filippo M et al. Photochemical Synthesis of Pyrazolines from Tetrazoles in Flow. SynOpen, **2022**. doi: [10.1055/a-1995-1859](https://doi.org/10.1055/a-1995-1859).

The Guiry group have published a book chapter "Asymmetric allylic alkylation and related reactions", Laura Cunningham, Vivek Sundaravel and Patrick J. Guiry, *Comprehensive Chirality*, 2nd edition and a Review article in *Annual Review of Pharmacology and Toxicology*, Catherine Godson, Patrick Guiry & Eoin Brennan, *Annu. Rev. Pharmacol. Toxicol.* **2023**, *63*, [429](https://doi.org/10.1146/annurev-pharmtox-031922-01429).

Congratulation to the Brougham group, who had two papers accepted; one on the fundamentals of MRI contrast, congratulations to Eogan MacMahon MSc: *pH-dependence of MRI-contrast in magnetic nanoparticle suspensions demonstrates inner-sphere relaxivity contributions and reveals the mechanism of dissolution*, Eoghan MacMahon and Dermot F.

Brougham, Langmuir **2023**, <https://doi.org/10.1021/acs.langmuir.2c02621> (not available just yet)

and

one on a new material and with preclinical evaluation for pancreatic cancer, congrats to Cara Moloney PhD: *Long-circulating magnetoliposomes as surrogates for assessing pancreatic tumour permeability and nanoparticle deposition*, Cara Moloney, Tista Roy Chaudhuri, Joseph A. Spornyak, Robert M. Straubingerb, Dermot F. Brougham, Acta Biomaterialia, **2023** <https://doi.org/10.1016/j.actbio.2022.12.057>

## Events and Activities

Marcus Baumann gave keynote lectures on the topic of continuous flow photochemistry towards sustainable synthesis - at the Atlantic Basin Conference in Marrakech (Dec. 2022) and the 44th SACI meeting in Stellenbosch (Jan. 2023).

Elaine O'Reilly gave a research talk at '*Rising Stars in Organic Synthesis*' organised by Thieme WebCheminar.

Pat Guiry, Susan Quinn and Elaine O'Reilly were part of the judging panel for the Chemistry, Physics and Mathematics category in the BT Young Scientist and Technology Exhibition in January.

Pat Guiry has been appointed panel Member of CINNTE review of UCC (to be held in March 2023).

## Save the Date!

**January 31<sup>st</sup>:** ChemSoc are hosting a Start of Term Mixer in Farmer Browns Clonskeagh Tuesday the 31st of January at 7pm. We hope to see you all there!

**February 8<sup>th</sup>:** A breakfast, "Celebrating Women in Science", is being organised by the PostDocs and EDI Committee in the School, to mark *International Day of Women and Girls in Science*. The breakfast will take place University Club from 9.30am. All PhDs, postdocs and academic staff are invited, a link for eventbrite registration will be circulated shortly.

**March 15<sup>th</sup>:** Postdoc research seminar from **1-2pm**. Talks will be given by Adrià Martínez Aviñó and Mandapati Bhargava Reddy. Venue tbc.

**March 22<sup>nd</sup>:** A STEM Research Day for Academic staff, will take place on March 22<sup>nd</sup>, and is an all-day event. Further details will be confirmed soon.

**March 31<sup>st</sup>:** An event to mark International Women's Day "Not Just the 8<sup>th</sup> of March 2.0" will take place in the UCD cinema on March 31st. More information will follow soon.

**April 27<sup>th</sup>:** ChemSoc's Inaugural Lecture will take place on April 27<sup>th</sup> - time to be confirmed. Remember, Postdoc coffee mornings **every Tuesday at 9.30 am** in the first floor kitchen.