

# LIST OF PhD SPEAKERS, SEMINAR TITLES and PRINCIPAL INVESTIGATORS

## Theatre D Wednesday

### 9.30-11.0 Organic Synthesis

Cian Reid	UCD	Pat Guiry	Novel Axially Chiral P,N Ligands and their Applications within Asymmetric Catalysis
Sheila Fitzgerald	RCSI	Donal O'Shea	Chirality Through Double Click Reactions with Sondheimer Diyne
Ashis Dhara	NUIG	Paul Murphy	Design, Synthesis and Biological Evaluation of Galectin Inhibitors
Alex Gibney	DCU	Andrew Kellet	Click and Cut: Towards the Simplified Preparation of Cu(II) Chemotherapeutics

### 11.30-1.00 Reaction Mechanism

Joshua O'Donnell	UCC	Peter Byrne	Development of a New Rationale to Account for Selectivity in Reactions of Ambident Nucleophiles
Gavin Lennon	QUB	Paul Dingwall	Insights into the Mechanism and Origin of Selectivity in PalladiumCatalysed Carbene Insertion Cross-Coupling Reactions
Lorna Doyle	TCD	Aidan McDonald	Activation of an Mn <sup>II</sup> Mn <sup>III</sup> -Peroxide with Relevance to the Catalytic Cycle of Ib RNRs
Sadbh Byrne	UCD	Declan Gilheany	Enantioselective Grignard Reactions in Total Synthesis: Development of Asymmetric Methodology and Exploration of New Targets

### 2.00-3.00 Biological Activity

Eoin Hever	NUIG	Paul Murphy	Design, Synthesis and Biological Evaluation of Galactosidase Inhibitors
Mark Stitch	UCD	Susan Quinn	Combining Spectroscopic techniques to Unravel the Binding of an Osmium Polypyridyl Probe to G-quadruplex Structures in Solution
Caytlin Boylan	MU	John Lowry	Monitoring Acetylcholine and Choline using Electrochemistry

## Theatre E Wednesday

### 9.30-11.00 Materials 1

Aisling Fleming	UCD	Kenneth Dawson	Particle Mapping by Fluorescence Microscopy: Characterizing Surface Composition and Subpopulation Heterogeneity of Bionanocomposites
Yaoguang Song	QUB	Xiaolei Zhang & Peter Nockemann	Ionic liquid-assisted Synthesis of Mesoporous Carbons for Supercapacitors
Reabetswe Zwane	DCU	Joaquin Klug	The Elastic Properties of Postulated Solid Forms from First Principles
Nilotpai Kapuria	UL	Kevin Ryan	Metal Seed Chemistry to Control Growth of Multicomponent Metal Chalcogenide Nanocrystals

### 11.30-1.00 Materials 2

Vivek Christhunathan	NUIG	Mingming Tong	<i>Ab-initio</i> Modelling on the Electronic and Absorption Properties of Pure and Cu-Doped $\text{CaWO}_4$
Anthony Dodd	QUB	Peter Nockemann	Multidentate Amide Ligands for the Separation of Rare Earth Elements
Mohini Mishra	UL	Kevin Ryan % Shalini Singha	Colloidal Synthesis of Copper Telluride using Diphenylditelluride as Alternative Te Source
Yiming Huang	QUB	Steven Bell	Controlling Nanoparticle Aggregates for Stable SERS

### 2.00-3.00 Chemical Imaging

David Cullinane	DCU	Tia Keyes	Drug Delivery Technology for Cell Permeation of Novel Luminescent Ruthenium Polypyridyl Complexes for Cell Imaging & Therapeutics
Colm McKeever	MU	Eithne Dempsey	Latent Fingerprint Enhancement on Brass Substrates with the aid of Electrochromic and Redox Polymer Deposition
Niamh Curtin	RCSI	Donal O'Shea	Exploiting Directed Self-Assembly and Disassembly for off-to-on Fluorescence Responsive Live Cell Imaging

## Theatre D Thursday

### 9.30-11.00 Flow Chemistry

Cormac Bracken	UCD	Marcus Baumann	The Photoflow Generation and Capture of Reactive Intermediates
Ailbhe Ryan	QUB	Mark Muldoon	Development of a Continuous Flow Process for the Epoxidation of Alkenes with Peracetic Acid and a Homogeneous Manganese(II) Catalyst
Lara Nolan	QUB	Peter Knipe	Continuous Synthesis of $\alpha$ -Substituted Cyclic Amines via C-H Functionalization Reactions
Aoife Kearney	UCC	Stuart Collins & Anita Maguire	Using Batch and Continuous Flow for the Synthesis of $\alpha$ -Sulfonyl- $\beta$ -chlorolactams

### 11.30-1.10 CO<sub>2</sub> Chemistry

Florian Cerpentier	DCU	Mary Pryce	The Design and Study of Novel Ruthenium Supramolecular Assemblies for Photocatalytic Hydrogen Evolution and CO <sub>2</sub> Reduction
Kristy Stanley	UCD	James Sullivan	New Vistas of an Old Reaction
Daniel Kerr	DCU	Brian Kelleher	A Python Based Non-Linear Regression Model to Estimate Acid-Base Characteristics of Organic Alkalinity – Pilot Study Dublin Bay
Qi Huang	QUB	Chunfei Wu	Enhanced Efficiency of a Photo Switching Metal-Organic Framework Toward Low Energy Carbon Dioxide Capture
Amy Bridget Lowry	UCC	Peter Byrne & Gerard McGlacken	Synthesis of $\alpha,\beta$ -Unsaturated Carboxylic Acids by Phosphonium Ylide-Mediated CO <sub>2</sub> Activation

## Theatre E Thursday

### 9.30-11.00 Medicinal Chemistry

Cathal Caulfield	RCSI	Donal O'Shea	Synthesis and Testing of Water-Soluble Near Infrared Azadipyrrromethene (NIR-AZA) Fluorophores
Karolina Wojtczak	NUIG	Joseph Byrne	Shining a Light on Bacteria: Lanthanide-Based Glycoconjugate Molecular Sensors for Lectins
Hua Tong	MU	Robert Elmes	Squararides: A New Family of Macrocyclic Peptidomimetics with Application as Anion Recognition Scaffolds
Liam Fitzgerald	NUIG	Paul Murphy	Docking of Sialic Acid Derivatives to Influenza Hemagglutinin and Synthesis of Glycoclusters Based on a Tetraphenylethylene Scaffold

### 11.30-1.10 Therapeutic Agents

Ioannis Titilas	NUIG	Luca Ronconi	Metal-based Glycoconjugates for Targeted Anticancer Chemotherapy
Neville Murphy	NUIG	Pau Farràs	Metallacarboranes: a Versatile New Player in Biomedicine
Ashutosh Sharma	SETU	Helen Hughes	Novel Process Strategies for the Stabilization of Biopharmaceuticals for Parenteral Use
	Waterford		
Avelino Ferreira	RCSI	Marco Monopoli	In vitro and In vivo Biological Evaluation of Functionalized Ultrasmall Gold Nanoparticles for Targeted Drug
Erika Mooney	TUD	Bernie Creaven & Fintan Kelleher	Synthetic Strategies towards Improving the Solubility Profile of Novel Antimicrobial Coumarin Derivatives

## LIST OF POSTER PRESENTERS, TITLES and PRINCIPAL INVESTIGATORS

No	Name	Univ	Principal Investigator	Poster Title
1	Aaron McCormack	NUIG	Paul V. Murphy	New Prospects of Carbohydrates as Chiral Auxiliaries for Tandem Cycloaddition Reactions: Batch vs Flow
2	Aidan Cregan	UCC	Peter Byrne	H-Phosphonate-Promoted Halogenation of Alcohols using Lithium Halides
3	Aine Coogan	TCD	Yurii Gun'ko	Chiroptically Active Copper Oxide Microstructures via Post-Synthetic Treatment of Copper-Aluminium Layered Double
4	Aisling Fleming	UCD	Kenneth Dawson	Development of an Immunogold Mapping Strategy to Unravel the Biomolecular Architecture of Bionanocomposite Materials
5	Aleksandra Krajewska	TCD	Aidan McDonald	Synthesis of Negatively Charged 2D 2H-MoS <sub>2</sub> and Its Functionalization
6	Alice Parkes	UL	Emmet O'Reilly & Gavin Walker	Controlling the Polymorphism of Carbamazepine by Droplet-Confinement via Spray Drying
7	Amit Upadhyay	UCC	Timothy O'Sullivan	Development of a Synthetic Route to Novel IMPDH Inhibitors
8	Andreea Cislaru	MU	Roisin O'Flaherty	Characterisation of Serum IgG Glycosylation in Cystinosis
9	Ashis Dhara	NUIG	Paul V. Murphy	Design and Synthesis of Carbohydrate Based Galectin Inhibitors
10	Cathal Kelly	QUB	Stuart James	Scrambled Macrocycles for Greener Porous Liquids
11	Ciara Davis	TUS	Peter Downey	Effects of selenium Application on Growth and Selenium Uptake in Lettuce.
12	Ciara Tyner	UCC	Stuart Collins & Anita Maguire	Studies in Intramolecular Buchner Reactions
13	Clara Evans	MU	Denise Rooney & Frances Heaney	Stability and Biological Activity of Novel Silver-based Antifungals to Avoid Antimicrobial Resistance
14	Conor Geraghty	MU	Robert Elmes	The Design and Synthesis of Ruthenium (II) Polypyridyl Complexes as Luminescent Probes for Nitroreductase

15	Conor Shine	RCSI	Marc Devocelle	The Development of PEG-based Antimicrobial Peptidomimetics
16	Dara Curran	UCC	Peter Byrne	Phosphorus-based Reductive Etherification of Aldehydes
17	Darren Beirne	MU	Diego Montagner & Trinidad V-Torrijos	Development of Dual-action Pt(IV)-Tyrosine Kinase Inhibitor Pro-drug Conjugates Targeting Colorectal Cancer
18	David Ryan	UCC	Peter Byrne	A New Rationale to Describe Ambident Reactivity
19	Eimear Courtney	UCC	David Jones & Gerard McGlacken	Application of a Supported Manganese Catalyst in C-H Activation and Reductive Transformations
20	Eoghain Murphy	MU	Eithne Dempsey	Dexamethasone Electroanalysis by Deposition of Copper on Glassy Carbon Electrodes with Quantitation in
21	Eoin Hever	NUIG	Paul V. Murphy	Design, Synthesis and Biological Evaluation of Galactosidase Inhibitors
22	Eoin Moynihan	MU	Diego Montagner & Trinidad V-Torrijos	Click-Pt(IV)-carbohydrate Pro-drugs for Treatment of Osteosarcoma
23	Eva Naughton	UCD	James Sullivan	Development of Cu <sub>2</sub> O/Ag <sub>3</sub> PO <sub>4</sub> Heterojunction Photocatalysts for Conversion of CO <sub>2</sub> into Fuels.
24	Farhad Mohammed	MU	Robert Elmes	Towards the Design and Synthesis of a New Biomimetic Code: Squaratic Acids
25	Foteini Dimakopoulou	NUIG	Constantina Papatriantafyllopoulou	Novel Co <sub>5</sub> and Ni <sub>4</sub> Metal Clusters by the Combination of 2-Pyridyl Oximes with Polycarboxylic Ligands
26	Hannah McKeever	UL	Shalini Singh	Colloidal Synthesis of Copper Bismuth Selenide Nanocrystals as Ionic Semiconductors for Photovoltaic Absorbers
27	Hilal Kirpik	MU	Robert Elmes	A New 3-Substituted BODIPY dye: Synthesis, Crystal Structure, and Photophysical Properties
28	Hugh Mohan	DCU	Silvia Giordani	Supramolecular Functionalisation of B/N Co-doped Carbon Nano-onions for Theragnostic Applications
29	Jack Bennett	NUIG	Paul V. Murphy	Applying Continuous Flow Techniques in the Synthesis of Sugar-based Therapeutics
30	Jacqueline Smyth	RCSI	Donal O'Shea	Exfoliation and Surface Functionalisation of Graphene in Water

31	Justynne Joy Fabian	TUD	Brendan Duffy	Surface Modification of Titanium Alloys for Biomedical Applications
32	Kate Donaghy	UCD	Eoghan McGarrigle	Stereoselective Synthesis of $\alpha$ -Galactosides
33	Kathryn McCarthy	NUIG	Pau Farràs	Two-Dimensional Porphyrin-Based Covalent Organic Frameworks as Photosensitizers for Light-Driven CO <sub>2</sub> Reduction
34	Keane Mc Namee	MU	John Lowry	The Development and Characterisation of a Biosensor for the Real-time Neurochemical Monitoring of Lactate
35	Keelan Byrne	MU	Tobias Krämer	Quantum Chemical Study of Low-Valent Aluminium Compounds
36	Kishan Mandal	NUIG	Paul V. Murphy	Design and Synthesis of Sialyl Triazoles as Siglec-8 Ligands
37	Kyle Doherty	MU	Trinidad Velasco-Torrijos	Development of Norbornene-based Compounds with Proposed Synergistic Anti-biofilm and Anti-adhesion Activities
38	Laura Foley	UL	Emmett O Reilly	Developing a Roadmap to Effective Spray Drying of Biomolecules
39	Lauren Kearney	DCU	Mary T. Price	A Photocatalytic & Electrocatalytic Investigation into Rhenium Tricarbonyl N-Heterocyclic Carbene Complexes for CO <sub>2</sub>
40	Levente Nagy	NUIG	Pau Farràs	Biphenyl Bridging Ligands as Building Blocks for Photoluminescent One-dimensional Gold Coordination Polymers
41	Lewis More O Farrell	TUD & RCSI	Christine O'Connor & Darren Griffith	Next-Generation Gallium Complexes to Combat Antimicrobial Resistance
42	Liam Fitzgerald	NUIG	Paul V. Murphy	Outcome of Docking of some Simple Sialic acid Derivatives to Influenza Hemagglutinin and Synthesis of Glycocluster
43	Lorna Doyle	TCD	Aidan McDonald	Activation of a Mn <sup>II</sup> Mn <sup>III</sup> -Peroxide with relevance to the Catalytic Cycle of Ib RNRs
44	Luke Brennan	MU	Robert Elmes	A Supramolecular Approach to Anti-Microbial Resistance: Anionophores that Induce Disruption of Bacterial Chloride Homeostasis
45	Mairéad Gallagher	TUD	Fintan Kelleher	Antibiotic Metabolites: Synthesis and Characterisation of the Human Metabolites of Ciprofloxacin
46	Manting Mu	TCD	Max García-Melchor.	Mechanistic Insights into the Ferration of Aromatic Substrates via Intramolecular Sodium Mediation

47	Maria Zubair	UL	Kevin M. Ryan & Shalini Singh	Compositionally Tunable Cu-Sb-M-S (M= Zn, Co and Ni) Nanocrystals: Synthesis and their Transport Properties
48	Marie Clara Michel	UCC	Peter Byrne & Gerard McGlacken	One Pot Tandem Wittig Hydrogenation Reactions to form C(sp <sup>3</sup> )-C(sp <sup>3</sup> ) in Water
49	Martina Tuberti	TUD	Fintan Kelleher	Computational Studies in Human Tau Protein Screening for Understanding the Impact in Alzheimer's disease
50	Martyna Bartusiak	DCU	Mary T. Price	A Time-Resolved Spectroscopic Analysis of Novel Porphyrins and Utilisation of their Aggregation in Dye-sensitized Solar Cells
51	Mary Hennessy	UCC	Timothy O Sullivan	Preparation of 1,2-Dioxolanes via the Enantioselective Peroxidation of $\gamma,\delta$ -Unsaturated- $\beta$ -Keto Esters
52	Michal Bartkowski	DCU	Silvia Giordani	Smart Carbon Nano-onion Systems for Drug Delivery
53	Mona Alanazi	NUIG	Constantina Papatriantafyllopoulou	Novel Mixed-Ligand Coordination Polymers and Metal-Organic Frameworks
54	Niraj Nitish Patil	UL	Kevin M. Ryan & Shalini Singh	Tuning Polytypism in Transition Metal Disulphides by Precursor Reactivity Manipulation and Application in
55	Palina Bruyek	TUD	Reeta Joshi & Mary Deasy	Development of Calixarene Based Surface Imprinted Polymer as a Novel Scavenging Device for Biological Contaminants in Water
56	Paul O'Dowd	RCSI	Darren Griffith	Exploiting Inverse Electron-demand Diels-Alder Click Chemistry for the Functionalisation of a Pt-based Anticancer Drug
57	Qinglu Chen & Heather McDonald	QUB	Steven Bell	SERS Analysis of Organic Extractants using 2D Hydrogel-based Nanoparticle Arrays
58	Rachel Lynch	UCC	Peter Byrne	Carbon Dioxide Utilisation for Construction of High Value CarboxylContaining Organic Products and Biologically Active Compounds
59	Raphaël Abolivier	UCD	James Sullivan	Catalytic Approaches to the Valorisation of Lignin
60	Rebecca Lynch	UCD	Declan Gilheany	Development of the Catalytic Asymmetric Grignard Synthesis of Tertiary Alcohols
61	Riddhi Salotra	QUB	Pamela J Walsh.	Quantitative Estimation of Total Phenolic Content in Brown Seaweeds through <sup>1</sup> H NMR Spectroscopy
62	Robert Fox	DCU	Joaquin Klug	Stability of Co-crystals: a Density Functional Theory Study



63	Shan Huang	UCC	Simon Lawrence	Pharmaceutical Salts of Piroxicam and Meloxicam with Organic Counterions
64	Shane Grant	NUIG	Alan Ryder	Elemental Screening of Cell Culture Media using Microwave Plasma Atomic Emission Spectroscopy
65	Simon Poole	DCU	Andrew Kellet	Development of Holliday Junction-stabilising complexes via Click Chemistry: a new Gene Targeting Strategy for Metal-based Drugs
66	Siobhán O'Flaherty	RCSI	Marc Devocelle	Synthesis of Cholesterol-Modified Antimicrobial Peptides
67	Tara Barwa & Yiran Luo	MU	Carmel Breslin	Development of a Bismuth Modified Molybdenum Disulfide Sensor for the Detection of Antibiotic Drugs in Water
68	Usaid Azhar	ATU Sligo	Ioannis Manolakis	Synthesis and Characterization of PEG <sub>400</sub> -DOPA for Multifunctional Coatings
69	Vanessa Becker	UCD	Eoghan McGarrigle	Bis-heteroaryl Synthesis via Pyridylsulfonium Salts
70	Xuan-Manh Pham	UL	Kevin M. Ryan	The Inverted Device Fabricated by Electrophoretic Deposition with high Luminescence and high EQE
71	Xuanyang Luo	MU	Robert Elmes	Probing the Metal Binding Characteristics of Squaramides
72	Yingrui Zhang	QUB	Yikai Xu	Surface-accessible Plasmonic Pickering Emulsions as Substrates for Direct SERS Analysis in Bio-media

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## Theatre E Wednesday

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Nilotpai Kapuria	UL	Kevin Ryan	Metal Seed Chemistry to Control Growth of Multicomponent Metal Chalcogenide Nanocrystals

### 11.30-1.00 Materials 2

Vivek Christhunathan	NUIG	Mingming Tong	<i>Ab-initio</i> Modelling on the Electronic and Absorption Properties of Pure and Cu-Doped $\text{CaWO}_4$
Anthony Dodd	QUB	Peter Nockemann	Multidentate Amide Ligands for the Separation of Rare Earth Elements
Mohini Mishra	UL	Kevin Ryan % Shalini Singha	Colloidal Synthesis of Copper Telluride using Diphenylditelluride as Alternative Te Source
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Aoife Kearney	UCC	Stuart Collins & Anita Maguire	Using Batch and Continuous Flow for the Synthesis of $\alpha$ -Sulfonyl- $\beta$ -chlorolactams

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Daniel Kerr	DCU	Brian Kelleher	A Python Based Non-Linear Regression Model to Estimate Acid-Base Characteristics of Organic Alkalinity – Pilot Study Dublin Bay
Qi Huang	QUB	Chunfei Wu	Enhanced Efficiency of a Photo Switching Metal-Organic Framework Toward Low Energy Carbon Dioxide Capture
Amy Bridget Lowry	UCC	Peter Byrne & Gerard McGlacken	Synthesis of $\alpha,\beta$ -Unsaturated Carboxylic Acids by Phosphonium Ylide-Mediated CO <sub>2</sub> Activation

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Ashutosh Sharma	SETU	Helen Hughes	Novel Process Strategies for the Stabilization of Biopharmaceuticals for Parenteral Use
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Avelino Ferreira	RCSI	Marco Monopoli	In vitro and In vivo Biological Evaluation of Functionalized Ultrasmall Gold Nanoparticles for Targeted Drug
Erika Mooney	TUD	Bernie Creaven & Fintan Kelleher	Synthetic Strategies towards Improving the Solubility Profile of Novel Antimicrobial Coumarin Derivatives