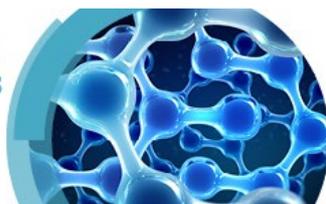


Harnessing non-covalent interactions for synthesis and catalysis

Faraday Discussion



12-14 April 2023
York, UK and online

Wednesday 12 April 2023 (all timings are BST)

12:00	Registration and lunch
12:45	Welcome and Introductions Andrew Weller, <i>Chair of Scientific Committee</i>
12:55	Outline of Discussion format Claire Mitchell and Michael Whitelaw, <i>Royal Society of Chemistry</i>
13:00	(Session chairs: Anne Duhme-Klair and Andrew Weller) Spiers memorial lecture - Introductory lecture Thomas Ward <i>University of Basel</i>
	Session 1: Make – underpinning concepts of the synthesis of systems where non-covalent interactions are important (Session chairs: Joost Reek and Neil Champness)
14:00	Fine-tuning non-covalent interactions between hybrid metal-oxo clusters and proteins Tatjana Parac-Vogt <i>KU Leuven</i>
14:05	Effect of liquid confinement on regioselectivity in the hydrosilylation of alkynes with cationic Rh(I) N-heterocyclic carbene catalysts Michael Buchmeiser <i>University of Stuttgart</i>
14:10	Discussion
15:00	Refreshments
	Session 1 continued (Session chairs: Neil Champness and Joost Reek)
15:30	Site-selective C-H oxidation of aliphatic protonated diamines enabled by supramolecular recognition using a manganese bioinspired catalyst Miquel Costas <i>Universitat de Girona</i>
15:35	Solution and solid-state studies of hydrogen and halogen bonding towards N-heterocyclic carbene supported nickel(II) fluoride complexes Torsten Beweries <i>LIKAT Rostock</i>
15:40	Chalcogen bonding in copper(II)-mediated synthesis Kamran Mahmudov <i>University of Lisbon</i>
15:45	Discussion
17:00	Flash poster presentations
17:30	Poster session and wine reception
19:00	Close of sessions

Thursday 13 April 2023 (all timings are BST)

	Session 2: Manipulate – techniques to manipulate the surroundings of a synthetic catalyst to control activity and selectivity (Session chairs: Anne Duhme-Klair and Joost Reek)
09:00	Catalytic templated length-controlled oligomerization Helma Wennermers <i>ETH Zürich</i>
09:05	The bridge towards a more stable and active side-on-peroxide ($\text{Cu}_2^{\text{II}}(\mu\text{-}\eta^2\text{:}\eta^2\text{-O}_2)$) complex as a tyrosinase model system Sonja Herres-Pawlis <i>RWTH Aachen</i>
09:10	On the mechanism of intermolecular nitrogen-atom transfer from a lattice-isolated diruthenium nitride intermediate David Powers <i>Texas A&M University</i>
09:15	Discussion
10:30	Refreshments
	Session 2 continued (Session chairs: Andrew Weller and Neil Champness)
11:00	A Substrate Descriptor Based Approach for the prediction and understanding of the Regioselectivity in caged catalyzed hydroformylation Pim Linnebank <i>University of Amsterdam</i>
11:05	Boosting the activity of Mizoroki-Heck cross-coupling reactions with a supramolecular palladium catalyst favoring remote Zn...pyridine interactions Rafael Gramage-Doria <i>CNRS University of Rennes</i>
11:10	Probing the influence of substrate binding on photocatalytic dehalogenation with a heteroleptic supramolecular $[\text{M}_4\text{L}^{\text{a}_2}\text{L}^{\text{b}_2}]$ square containing PDI photosensitizers as ligands Sonja Pullen <i>University of Amsterdam</i>
11:15	Discussion
12:30	Lunch
	Session 3: Model – state-of-the-art modelling and computational analysis of reactive sites (Session chairs: Andrew Weller and Paul Raithby)
13:30	A comparison of non-covalent interactions in the crystal structures of two σ-alkane complexes of Rh exhibiting contrasting stabilities in the solid state Stuart Macgregor <i>Heriot-Watt University</i>
13:35	Catalytic activation via π-backbonding in halogen bonds Pierre Kennepohl <i>University of Calgary</i>
13:40	H-Bonding leading to latent initiators for olefin metathesis polymerization Albert Poater <i>Universitat de Girona</i>
13:45	Discussion
15:00	Refreshments
	Session 3 continued (Session chairs: Paul Raithby and Andrew Weller)
15:30	Mapping the photochemistry of cyclopentadiene: From theory to ultrafast x-ray scattering Adam Kirrander <i>University of Edinburgh</i>
15:35	Alkali metal...methyl short contacts in aluminates and related compounds: More than just agostic interactions Jorge Echeverria <i>Universidad de Zaragoza</i>

15:40	Machine-learning based prediction of small molecule – surface interaction potentials Ian Rouse <i>University College Dublin</i>
15:45	Discussion
17:00	Close of sessions
18:00	Pre-dinner drinks
18:30	Conference dinner

Friday 14 April 2023 (all timings are BST)

09:00	Journal publishing Join authors, academic editors and RSC editors to discuss and gain insights in journal publishing. This session is aimed at Postgrads and ECRs but all delegates are very welcome and we encourage you to join us. Lauren Hatcher, <i>Cardiff University</i> Bianca Provost, Deputy Editor, <i>Royal Society of Chemistry</i> Andrew Weller, Associate Editor, <i>Catalysis Science & Technology</i>
	Session 4: Measure – understanding of structural and electronic changes occurring within the relevant timescale of catalytic systems (Session chairs: Paul Raithby and Anne Duhme-Klair)
09:30	Noncovalent bonding assessment by Pair Distribution Function Maria Diaz Lopez <i>Diamond Light Source</i>
09:35	Uncovering the role of non-covalent interactions in solid-state photoswitches by non-spherical structure refinements with NoSpherA2 Lauren Hatcher <i>Cardiff University</i>
09:40	Discussion
10:30	Refreshments
	Session 4 continued (Session chairs: Anne Duhme-Klair and Andrew Weller)
11:00	Ultrafast electronic, infrared, and X-ray absorption spectroscopy study of excited state dynamics of Cu(I) phosphine diamine complexes Julia Weinstein <i>University of Sheffield</i>
11:05	Structural Modifications to Platinum(II) Pincer Complexes Resulting in Changes in their Vapochromic and Solvatochromic Properties Paul Raithby <i>University of Bath</i>
11:10	Discussion
12:00	(Session Chairs: Joost Reek and Andrew Weller) Concluding remarks lecture Dean Toste <i>University of California, Berkeley</i>
12:40	Acknowledgements
12:45	Close of meeting and lunch