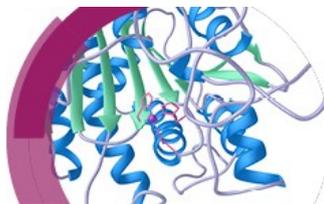


Natural and artificial metalloenzymes

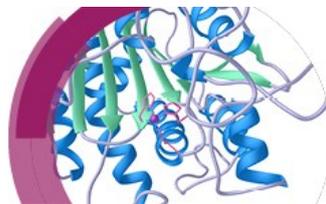
Faraday Discussion



31 January – 3 February 2022
Online

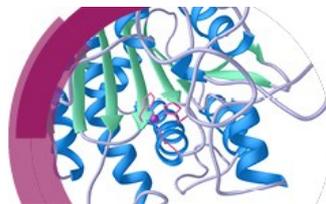
Monday 31 January (all timings in GMT)

16:00	Welcome and Introductions Rabindranath Mukherjee <i>IIT Kanpur, India</i>
16:10	Outline of Discussion Format Donna Smith and Eleanor Clifford <i>Royal Society of Chemistry Publishing Editors</i>
16:15	Introductory Lecture (Session Chair: Rabindranath Mukherjee and Sankar Rath) Edward Solomon <i>Stanford University, USA</i>
17:15	Close of sessions



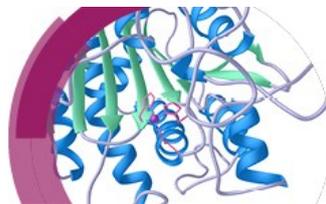
Tuesday 1 February (all timings in GMT)

	Session 1: Small molecule activation and synthetic analogues (Session Chair: Shinobu Itoh and Sankar Rath)
09:00	A bio-inspired heterodinuclear hydrogenase CoFe complex Carol Duboc <i>Université Grenoble Alpes, France</i>
09:05	Electrocatalytic Alcohol Oxidation by a Molecular Iron Complex Sayam Sen Gupta <i>IISER Kolkata, India</i>
09:10	Oxidative dehalogenation of halophenols by high-valent nonheme iron(IV)-oxo intermediates Chivukula Sastri <i>Indian Institute of Technology Guwahati, India</i>
09:15	Discussion
10:30	Poster session
11:30	Break
	Session 1 continued: Small molecule activation and synthetic analogues (Session Chair: Sankar Rath and Rabindranath Mukherjee)
15:30	Syntheses and investigation of metal complexes with macrocyclic polythioether ligands Siegfried Schindler <i>Justus-Liebig-Universität, Germany</i>
15:35	Phenolate-bonded bis(m-oxido)-biscopper(III) intermediates: hydroxylation and dehalogenation reactivities Dan Stack <i>Stanford University, USA</i>
15:40	Explorations of the nonheme high-valent iron-oxo landscape: crystal structure of a synthetic complex with an [FeIV2 (m-O)2] diamond core relevant to the chemistry of sMMOH Lawrence Que <i>University of Minnesota, USA</i>
15:45	Discussion
17:00	Close of sessions



Wednesday 2 February (all timings in GMT)

	Session 2: Electron transfer, spectroscopy and theory (Session Chair: Shinobu Itoh and Shyamalava Mazumdar)
09:00	O₂ reduction by iron porphyrins with electron withdrawing groups: to scale or not to scale Abishek Dey <i>Indian Association for the Cultivation of Science, India</i>
09:05	Comparative analysis of lanthanide excited state quenching by electronic energy and 1 electron transfer processes David Parker <i>Durham University, UK</i>
09:10	Can you break the oxo-wall? A multiconfigurational perspective Gopalan Rajaraman <i>IIT Bombay, India</i>
09:15	Discussion
10:30	Break
	Session 2 continued: Electron transfer, spectroscopy and theory (Session Chair: Sankar Rath and Rabindranath Mukherjee)
14:00	Binding of the Substrate Analog Methanol in the Oxygen-evolving Complex of Photosystem II in the D1-N87A Genetic Variant of Cyanobacteria K. V. Lakshmi <i>Rensselaer Polytechnic Institute, USA</i>
14:05	Enzymatic X-ray Absorption Spectroelectrochemistry Serena DeBeer <i>Max Planck Institute for Chemical Energy Conversion, Germany</i>
14:10	Intermediate-spin iron(IV)-oxido species with record reactivity Peter Comba <i>Heidelberg University, Germany</i>
14:15	Discussion
15:30	Poster session



Thursday 3 February (all timings in GMT)

	Session 3: Natural and artificial enzymes and medicinal aspects (Session Chair: Akhil R. Chakravarty and Shyamalava Mazumdar)
09:00	Density functional theory investigation of Ru(II) and Os(II) asymmetric transfer hydrogenation catalysts Peter Sadler <i>University of Warwick, UK</i>
09:05	A GPx-mimetic copper vanadate nanozyme mediates the release of nitric oxide from S-nitrosothiols G Mugesh <i>Indian Institute of Science, India</i>
09:10	Exploring hitherto uninvestigated reactions of the fatty acid peroxygenase CYP152A1: catalase reaction and compound I formation Osami Shoji <i>Nagoya University, Japan</i>
09:15	Discussion
10:30	Break
	Session 3 continued: Natural and artificial enzymes and medicinal aspects (Session Chair: Akhil R. Chakravarty and Debabrata Goswami)
11:00	Computational driven design of an artificial metalloenzyme using supramolecular anchoring strategies of iridium complexes to alcohol dehydrogenases Christof Jaeger <i>University of Nottingham, UK</i>
11:05	Mapping the protonation states of the histidine brace in an AA10 lytic polysaccharide monoxygenase using CWEP spectroscopy and DFT calculations Paul Walton <i>University of York, UK</i>
11:10	Successes and challenges in multiscale modelling of artificial metalloenzymes: the case study of POP-Rh2 cyclopropanase Jean-Didier Marechal <i>Universitat Autònoma de Barcelona, Spain</i>
11:15	Discussion
12:30	Break
14:00	Concluding Remarks lecture (Session chair: Debabrata Goswami and Sankar Rath) Kenneth Karlin <i>Johns Hopkins University, USA</i>
14:45	Acknowledgements
15:00	Close of meeting