

**Programme**  
**Faraday Discussion 148**  
**5 – 7 July 2010**  
**University of Nottingham, UK**

**Monday 5 July**

13:00	<b>Welcome and Introductions</b>
<b>Session 1</b>	Session Chair: Emma Raven, <i>University of Leicester</i>
13:15 <b>Paper 1</b>	<b>Introductory Lecture</b> Ed Solomon <i>Stanford University, USA</i>
14:15 <b>Paper 2</b>	<b>Reductive cleavage of the O-O bond in multicopper oxidases: QM/MM and QM study</b> Martin Srnec, Ulf Ryde and Lubomír Rulíšek* <i>Academy of Sciences of the Czech Republic, Czech Republic</i>
<b>Paper 3</b>	<b>Theoretical simulation of the spectroscopy and dynamics of a red copper protein</b> Nicholas A Besley* and David Robinson <i>University of Nottingham, UK</i>
15:15	<b>Afternoon Tea</b>
15:45 <b>Paper 4</b>	<b>Relating dynamic protein interactions of metallochaperones with metal transfer at the single-molecule level</b> Jamie J Benítez, Aaron M Keller, David L Huffman, Liliya A Yatsunyk, Amy C Rosenzweig and Peng Chen* <i>Cornell University, USA</i>
<b>Paper 5</b>	<b>Proton-coupled electron transfers in biomimetic water bound metal complexes. The electrochemical approach</b> Elodie Anxolabéhère-Mallart, Cyrille Costentin, Marc Robert* and Anne-Lucie Teillout <i>Université Paris Diderot, France</i>
16:45	<b>Close of Session</b>
17:00 – 18:30	<b>Poster Session</b>
19:30	<b>Dinner</b> – for delegates who have pre-booked in halls of residence, otherwise no formal arrangements.

Tuesday 6 July

<b>Session 2</b>	Session Chair: Rob Deeth, <i>University of Warwick</i>
09:00 <b>Paper 6</b>	<b>Comparison of QM-only and QM/MM models for the mechanism of tyrosinase</b> Per E M Siegbahn* and Tomasz Borowski <i>Stockholm University, Sweden</i>
<b>Paper 7</b>	<b>An enquiry into theoretical bioinorganic chemistry: how heuristic is the character of present-day quantum chemical methods?</b> Maren Podewitz, Martin T Stiebritz and Markus Reiher* <i>ETH Zurich, Switzerland</i>
<b>Paper 8</b>	<b>What can molecular modelling bring into the design of artificial inorganic cofactors?</b> Victor Muñoz Robles, Elisabeth Ortega-Carrasco, Eric González Fuentes, Agustí Lledós and Jean-Didier Maréchal* <i>Universitat Autònoma de Barcelona, Spain</i>
10:30	<b>Morning Coffee</b>
11:00 <b>Paper 9</b>	<b>Channeling of electrons within SLAC, the small laccase from <i>Streptomyces coelicolor</i></b> Armand W J W Tepper, Thijs J Aartsma and Gerard W Canters* <i>Leiden University, The Netherlands</i>
<b>Paper 10</b>	<b>Continuum electrostatic investigations of charge transfer processes in biological molecules using a microstate description</b> Elisa Bombarda and G Matthias Ullmann* <i>University of Bayreuth, Germany</i>
<b>Paper 11</b>	<b>How do enzymes reduce metals? : The mechanism of the reduction of Cr(VI) in chromate by cytochrome <i>c</i><sub>7</sub> proteins proposed from DFT calculations</b> Mahesh Sundararajan, Andrew J Campbell and Ian H Hillier* <i>University of Manchester, UK</i>
12:30	<b>Close of Session and Lunch/Posters</b>

<b>Session 3</b>	Session Chair: Julea Butt, <i>University of East Anglia</i>
14:00 <b>Paper 20</b>	<b>What is not required to make a single molecule magnet</b> Frank Neese and Dimitrios A Pantazis* <i>University of Bonn, Germany</i>
<b>Paper 13</b>	<b>Resonance Raman study on the oxygenated and the ferryl-oxo species of indoleamine 2, 3-dioxygenase during catalytic turnover</b> Sachiko Yanagisawa, Masaki Horitani, Hiroshi Sugimoto, Yoshitsugu Shiro, Norihiro Okada and Takashi Ogura* <i>University of Hyogo, Japan</i>
<b>Paper 14</b>	<b>Implications for the mechanism of sulfite oxidising enzymes from pulsed EPR spectroscopy and DFT calculations for "difficult" nuclei</b> John H Enemark*, Arnold M Raitsimring, Andrei V Astashkin and Eric L Klein <i>University of Arizona, USA</i>
15:30	<b>Afternoon Tea</b>
16:00 <b>Paper 15</b>	<b>Dissecting the mechanism of oxygen trafficking in a metalloenzyme</b> Mark A Smith, Peter F Knowles, Michael J McPherson and Arwen Pearson* <i>University of Leeds, UK</i>
<b>Paper 16</b>	<b>Prediction of nitroxide spin label EPR spectra from MD trajectories: application to myoglobin</b> Egidijus Kuprusevicius, Gaye White and Vasily S Oganessian* <i>University of East Anglia, UK</i>
17:00	<b>Close of Session</b>
19:00	<b>Pre-Dinner Drinks</b> Portland Building
19.30	<b>Conference Dinner</b> Portland Building

## Wednesday 7 July

<b>Session 4</b>	Session Chair: Jon McMaster, <i>University of Nottingham</i>
09:00 <b>Paper 17</b>	<b>Elucidating mechanisms in haem copper oxidases: The high-affinity Q<sub>H</sub> binding site in quinol oxidase as studied by DONUT-HYSCORE spectroscopy and density functional theory</b> Fraser MacMillan*, Sylwia Kacprzak, Petra Hellwig, Stephane Grimaldi, Hartmut Michel and Martin Kaupp <i>University of East Anglia, UK</i>
<b>Paper 18</b>	<b>Development of an infrared spectroscopic approach for studying metalloenzyme active site chemistry under direct electrochemical control</b> Adam J Healy, Holly A Reeve and Kylie A Vincent* <i>University of Oxford, UK</i>
<b>Paper 19</b>	<b>Protonation of (FeFe)-hydrogenase sub-site analogues: revealing mechanism using FTIR stopped-flow techniques</b> Joseph A Wright, Lee Webster, Aušra Jablonskytė, Pei Meng Woi, Saad K Ibrahim and Christopher J Pickett* <i>University of East Anglia, UK</i>
10:30	<b>Morning Coffee</b>
11:00 <b>Paper 12</b>	<b>Water as biocatalyst in cytochrome P450</b> Devesh Kumar, Ahmet Altun, Sason Shaik and Walter Thiel* <i>Max Planck Institut für Kohlenforschung, Germany</i>
<b>Paper 21</b>	<b>The quest for a functional substrate access tunnel in FeFe hydrogenase</b> Thomas Lautier, Pierre Ezanno, Carole Baffert, Vincent Fourmond, Laurent Cournac, Juan C Fontecilla-Camps, Philippe Soucaille, Patrick Bertrand, Isabelle Meynial-Salles and Christophe Léger* <i>CNRS Laboratoire de Bioénergétique et Ingénierie des Protéines, France</i>
<b>Paper 22</b>	<b>Fe-H/D stretching and bending modes in nuclear resonant vibrational, Raman and infrared spectroscopies: comparisons of density functional theory and experiment</b> Vladimir Pelmeshnikov, Yisong Guo, Hongxin Wang, Stephen P Cramer and David A Case* <i>Rutgers University, USA</i>
12:30 <b>Paper 23</b>	<b>Concluding Remarks</b> Les Dutton <i>University of Pennsylvania, USA</i>
13:00	<b>Acknowledgements</b>
13:15	<b>Close of Meeting</b>