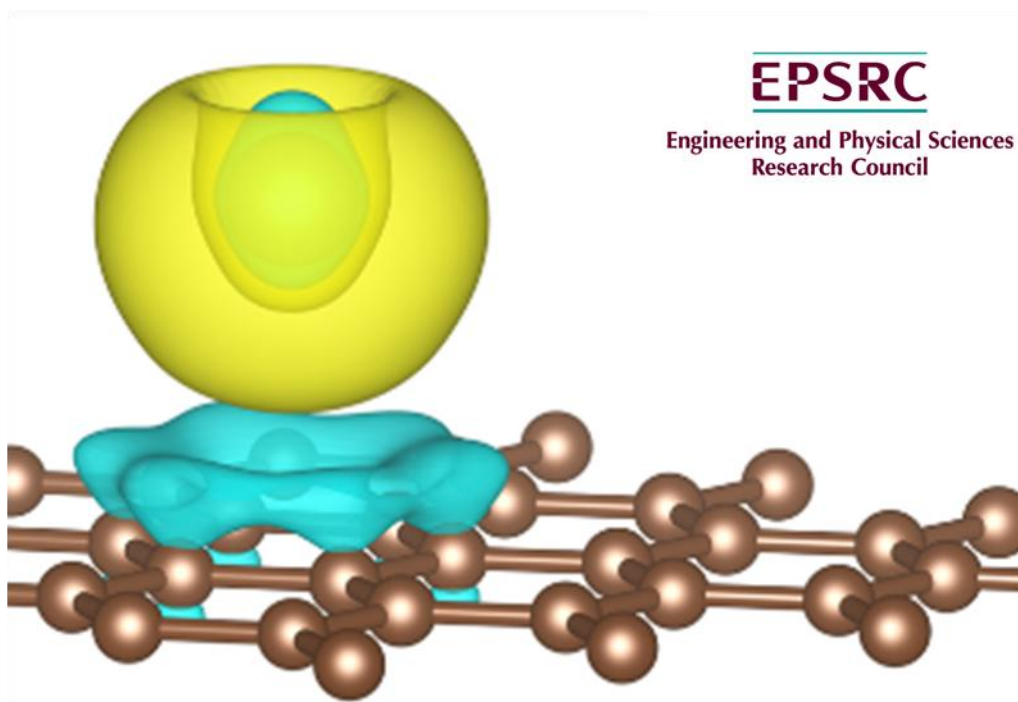


# MCC 2<sup>nd</sup> Conference



**Cardiff University**

Wednesday 6<sup>th</sup> April – Friday 8<sup>th</sup> April, 2016



## Sponsors

The MCC is very grateful for funding from EPSRC.

This event is also sponsored by:

Schools of Chemistry (both Cardiff and UCL)

Cardiff Catalysis Institute

## Organising Committee

David Willock, Richard Catlow and Scott Woodley

We also would like to thank all members, particularly those who helped us complete our recent report, our theme leaders and those of you, including our invited guests, who we will see at Cardiff.



Wednesday 6 <sup>th</sup> April		
13:50	Welcome	
Session 1:	Biomaterials	<b>Theme Leader</b> Jamieson Christie
14:00	<b>Invited:</b> All-electron Approach to the Microscopic Underpinnings of Energy Photo-Generation in Inorganic and Organic-Inorganic Hybrid Materials	Volker Blum Duke University
14:40	A Multinuclear Solid State NMR and GIPAW DFT Approach Towards the Evaluation of the Proposed Structural Motifs of Vaterite	Stephen P. Day Warwick (han)
15:00	Identification of Preferential Sites for Intra-molecular Advanced Glycation End Products Formation in Fibrillar Type I Collagen And Their Effect on the Function of Collagenous Tissues: An All Atom Molecular Dynamics Approach	Thomas A. Collier UCL (lee)
15:20	The Effect of Surface Chemistry on Protein Adsorption	Evangelos Liasas Birmingham (mul)
15:40	Tea	
Session 2:	Organic and Soft Matter	<b>(Chair and) Theme Leader</b> Graeme Day
16:00	Modelling Structural Transformations in Guest-Adaptable MOFs	Dmytro Antypov Liverpool (dar)
16:40	The Role of Solvent in the Self-Assembly of m-aminobenzoic acid: a Density Functional Theory and Molecular Dynamics Study	Etienne Gaines QMUL (dev)
17:00	<b>Invited:</b> Energy landscapes and nanomaterials	Christian Schön MPI Solid State R
17:40		
Session ends		
	Delegates put up posters	
18:00 – 20:00	Poster Session	

Thursday 7 <sup>th</sup> April		
Session 3:	Nano and Defect Chemistry	<b>Theme Leader</b> Alex Shluger
9:00	<b>Invited:</b> From Building Blocks to Bulk: Design and Understanding of Nanostructured Materials from the Bottom-up	Stefan T Bromley Barcelona University ICREA
9:40	The Identification and Passivation of Performance Limiting Defects in 4H-SiC Devices: From Bulk to the Interface and Beyond. An EDMR and ab initio Study	Jon Cottom UCL (shl)
10:00	Early Stages of Epitaxial Graphene Growth: Hydrocarbon Decomposition and Nucleation of Carbon Clusters	H. Tetlow KCL (lev)
10:20	Physical Properties of MgSiN <sub>2</sub>	Mikael Råsander Imperial (mor)
10:40	Defect and Band Engineering in Sn-based Oxides	David O. Scanlon Diamond (dos)

11:00	Coffee		
Session 4:	Surfaces and Interfaces	<b>Theme Leader</b> Ben Slater	
11:20	Enhancing the reducibility of CeO <sub>2</sub> : The role of divalent dopants	Aoife B. Kehoe Dublin (wat)	
11:40	Surface Composition of Magnesium and Calcium Rich Minerals	Marco Molinari Bath (par)	
12:00	Explaining the Stability of the Polar Surfaces of ZnO Using Interatomic Potentials	David Mora-Fonz UCL (cat)	
12:20	Numerical analysis of Pickering emulsion stability: insights from ABMD simulations	François Sicard UCL (str)	
12:40	Local electronic properties of Cu and its oxide clusters on CeO <sub>2</sub> surface	Arun Chutia Catalysis Hub (cat)	
13:00	Lunch		
Session 5:	Reactivity	<b>Chair and Theme Leader</b> David Willock	
13:50	Density Functional Theory Study of the Greigite (Fe <sub>3</sub> S <sub>4</sub> ) Surface to Bulk Oxidation	David Santos-Carballal Cardiff (lee)	
14:10	Formaldehyde Oxidation on Ytria-Stabilized Zirconia	Dominic T. Chaopradith UCL (cat)	
14:30	Adsorption and Diffusion of Aromatics on Metal Surfaces	Marco Sacchi Surrey (surfin-msa)	
14:50	A DFT Study of Free and Supported Au-Rh Nanoalloys	Ilker Demiroglu Bir'ham (surfin-roy)	
15:10	Coffee		
Session 6:	Environment	<b>Chair and Theme Leader</b> John Harding	
15:40	<b>Invited:</b> High Performance Computing in Southern Africa	Happy Sithole South Africa	
16:20	<b>Invited:</b> High Performance Computing for High Performance Science	Phil Hasnip UKCP, York	
17:00	Software for Structure Prediction at the Nanoscale	Tomas Lazauskas UCL (nandef-smw)	
17:20	Simulations of CO <sub>2</sub> Capture by Porous Metal-Organic Framework Materials	Martin T. Dove QMUL (dov)	
17:40	Yttrium Stabilised Cubic Zirconia	Chenxing Yang QMUL (kos)	
18:00	session ends		
19:30 – 22:00	Conference Dinner		

Friday 8 <sup>th</sup> April		
Session 7:	Energy Generation	<b>Chair and Theme Leader</b> Nic Harrison
9:00	Accelerated Discovery of Two New Structure Types in a Complex Inorganic Phase Field	C. Collins Liverpool (dar)
9:20	Accurate Exchange-correlation Energies for Warm Dense Matter	W.M.C. Foulkes Imperial (fou)
9:40	Optical Properties of Point Defects and Defect Complexes in GaN from Hybrid QM/MM	Zijuan Xie UCL (sok)
10:00	Simple Rules for Solid-state Design: From Bulk to Interface	Keith T. Butler Bath (wal)
10:30	Coffee	
Session 8:	Energy Storage	<b>Chair and Theme Leader</b> Saiful Islam
11:00	<b>Invited:</b> First-Principles Approaches to Understanding Kinetic Processes in Battery Electrodes	Anton van der Ven Santa Barbara
11:40	Band Gap Engineering of Iron Disulfide (FeS <sub>2</sub> ) for Photovoltaic Applications	Nelson Y. Dzade Utrecht University (gener-lee)
12:00	Path Sampling Adventures - Using High Performance Computing to Determine the Pathway, Mechanism and Energy Landscape of a Solid-Solid Phase Transition	Samuel A. Jobbins Cardiff (gener-leo)
12:20	Mechanisms of Li Extraction from Li-rich Layered Manganese Oxide Cathode Li <sub>2</sub> MnO <sub>3</sub>	Hungru Chen Bath (isl)
12:40	Dynamic Excitations in the Solid Lithium-Ion Electrolyte LLZO	Ben Morgan Bath (bjm)
13:00	Modelling Defect Microstructure in the Cathode Layer Material LaCoO <sub>3</sub>	John Buckeridge UCL (cat)
13:20	Final Remarks	