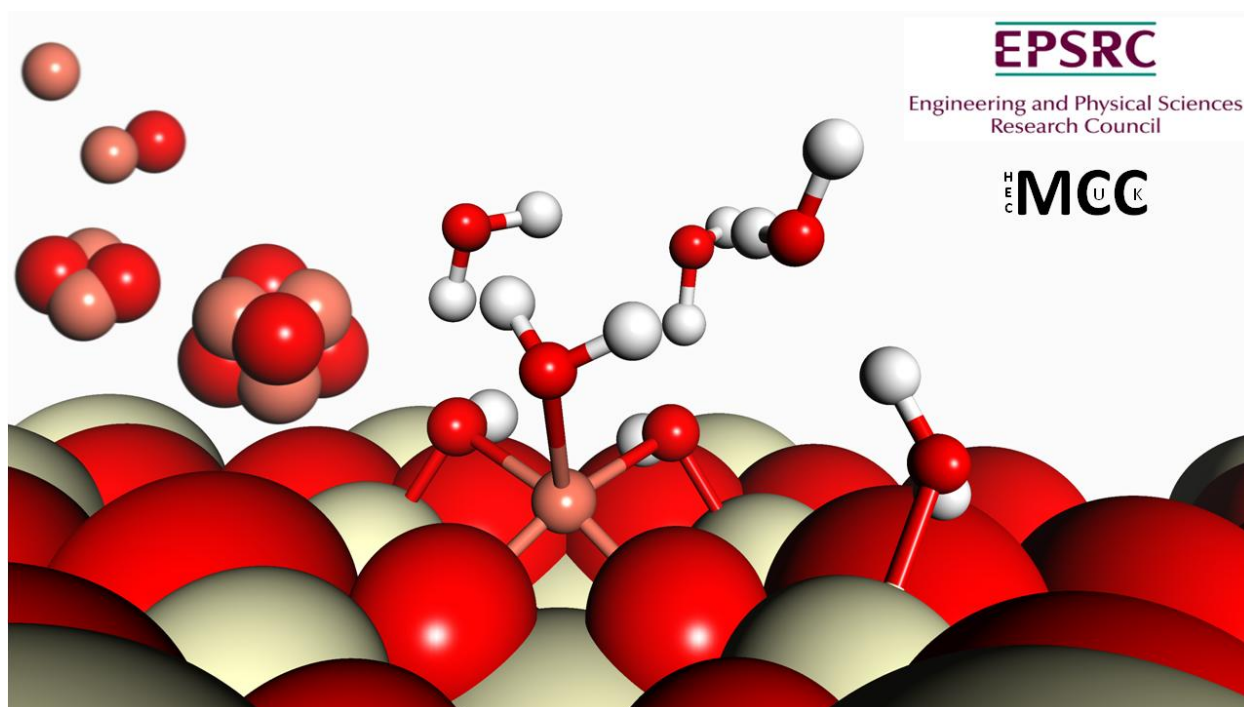


MCC 3rd Conference



Lincoln University

Monday 3rd September – Wednesday 5th September, 2018

Sponsors

The MCC is very grateful for funding from EPSRC.

We are grateful that this event is also sponsored by:

School of Mathematics and Physics (Lincoln)

School of Chemistry (Lincoln)

Department of Chemistry (UCL)

Organising Committee

Arun. Chutia, Matt. Watkins, Richard Catlow and Scott Woodley

We also would like to thank all members, particularly colleagues who have helped us complete our recent EPSRC proposal, our theme leaders and all of you, including our invited guests, who have joined us in Lincoln.

Monday 3 rd September		
09:30	Software Workshop	Isaac Newton Building
	Presentations and hands-on sessions with Scott Woodley (WASP@N), Volker Blum (FHI-aims), Julian Gale (GULP), Tom Keal (CHEMSHELL), Stewart Clarke (CASTEP), Matthew Watkins (CP2K)	
12:30	Registration Desk Open	Isaac Newton Building
13:00	Lunch	13:50 Start – Welcome Address
Session 1:	Minerals and Biomaterials	Theme Leader Jamieson Christie
14:00	Invited: Simulation of mineral speciation in aqueous solution	Julian Gale Curtin Uni, Perth
14:40	Early Oxidation of Prismatic Surfaces of Troilite FeS	Umberto Terranova Cardiff (surfin-lee)
15:00	Simulating the Effect of Organic Molecules on Clustering in Calcium Carbonate and Phosphate	John Harding Sheffield (har)
15:20	DL_POLY/FIELD – code overview, new developments, parallel performance and a few examples of applications	Chin Yong COSEC
15:40	Tea	
Session 2:	Organic and Soft Matter	Theme Leader Graeme Day
16:10	Invited: Order-disorder Interplay and Piezochromic Effects in Nanocrystals under Pressure	Carla Molteni KCL, London
16:50	Bulk and surface properties of metal carbides: implications for catalysis	Fabrizio Silveri Cardiff (cat)
17:10	Control of Pickering emulsion to advance new materials and knowledges	François Sicard UCL (surfin-str)
17:30	The Cluster-assembled Nanowires based on (XY) ₁₂ (X=Zn, Ga, Al, Y=O, N) Clusters as High Performance Gas Sensors	Yongliang Yong Hean University, China (cat)
17:50	Poster Session Starting with lightning presentations (1 slide per poster)	
20:00	Session ends	

Tuesday 4 th September		
Session 3:	Nano and Defect Chemistry	Theme Leader Alex Shluger
9:00	Invited: Precisely Tunable Materials with Help from Accurate Electronic Structure Theory - Where We Are and Where We Are Going	Volker Blum Duke University
9:40	First-principles modelling of polaron formation in TiO ₂ polymorphs	Razak Elmaslmane York (mck)
10:00	Relation between image charge and potential alignment corrections for charged defects in periodic boundary conditions	Thomas Durrant UCL (shl)
10:20	Ab initio design of ternary Sb-containing transparent conducting oxides	Adam Jackson UCL (dos)
10:40	Role of Carrier Injection and Localization in Degradation of Oxide Films	Alex Shluger UCL (shl)

11:00	Coffee		
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Session 4:	Surfaces and Interfaces	Theme Leader Ben Slater	
11:20	A DFT study of copper oxides as photovoltaic absorbers	Aleksander Zivkovic Cardiff (lee)	
11:40	Computational Studies of Porous Materials: from Defective Metal-Organic Frameworks to 2D Zeolites	Sanliang Ling Nottingham (lin)	
12:00	Pt-water Double Layer Structure in Realistic Solution Conditions	Clotilde Cucinotta Imperial (clo)	
12:20	The Interaction of Phosphate with Cerium Dioxide Surfaces	Macro Molinari Huddersfield (mol)	
12:40	CHEMSHELL – code overview, new developments, parallel performance and a few examples of applications	Tom Keal COSEC	
13:00	Lunch		
Session 5:	Reactivity	Theme Leader David Willock	
13:50	Computational QM/MM studies of the Methanol to Hydrocarbons process on zeolites H-Y and H-ZSM-5	Stefan Nastase Cardiff (log)	
14:10	Theoretical Simulation of the Catalytic CO ₂ Activation and Dissociation on the Major Magnetite Fe ₃ O ₄ Surfaces	Abdelazziz Cadi Cardiff (lee)	
14:30	Kinetic Control of Molecular Assembly on Insulating Surfaces	Andrea Floris Lincoln (flo)	
14:50	The Effect of Ceria Morphology on Gas Phase Glycerol Conversions	Mala Sainna Cardiff (wil)	
15:10	Coffee		
Session 6:	Environment and QM/QC	Chair and Theme Leader John Harding	
15:40	Invited: Computational Chemistry : An Industrial Perspective	Misbah Sarwar Johnson Matthey	
16:20	Hazardous Compounds at the Soil-Water Interface	Leyorla Ohene-Y Bath (surfin-par)	
16:40	Actinyl Adsorption on Magnetite (111)	Adam Thetford Manchester (surfin-nik)	
17:00	Hybrid Time Dependent Density Functional Perturbation Theory in CP2K	Sergey Chulkov Lincoln (nandef-mat)	
17:20	Invited: Quantum Computing and its Prospects for Computational Chemistry and Material Science	Matthew Hutchings SeeQC	
18:00	session ends		
19:00 – 22:00	Conference Dinner		Double Tree Hilton

Wednesday 5 th September		
Session 7:	Energy Generation	Theme Leader Nic Harrison
9:00	Photocatalytic Interfaces of TiO ₂ with Graphene and Reduced Graphene Oxide: A Computational Study	Natalia Martsinovich Sheffield (nat)
9:20	Insights into Emerging Photovoltaic Materials through Density Functional Theory	Christopher Savory UCL (dos)
9:40	Phonon Anharmonicity in Energy Materials	Jonathon Skelton Bath/Manchester (par/ske)
10:00	First-principles Study of Electronic and Structural Properties of CuFeO ₂ Surfaces	Lars Blumenthal Imperial (lis)
10:20	Coffee	
Session 8:	Energy Storage	Theme Leader Saiful Islam
11:00	Invited: Exchange interactions in solids	Stewart Clarke Durham (UKCP)
11:40	Computational Studies of Cathode Materials for Mg Ion Batteries	Kit McColl UCL (cor)
12:00	Doubled Conductivity in Transparent Conducting In ₂ O ₃ through Novel Dopant Design	Ben Williamson UCL (nandef-dos)
12:20	Global Optimisation of Alkali Earth Oxide Nanoclusters and their deposition on Graphene	Susanne Escher UCL (smw)
12:40	CRYSTAL – code overview, new developments, parallel performance and a few examples of applications	Barry Searle, COSEC
13:00	Final Remarks and Close	
TBA: Standby Talk	Structural Diversity of Quasi 1D Zinc Oxide: A Global Optimisation Approach	Scott Woodley, UCL (smw)