MCC 7th Conference - Programme

Monday 7rd July			
11:30	**Registration Desk Open**		**Daresbury Laboratory**
12:00	**Lunch**		
Session 1:	Power / Discovery	**Chair** Richard Catlow	
13:30	Suppressing phase transformation and cation migration with Mg and Si doping in Fe–Mn layered oxides for sodium-ion cathodes		Arup Chakraborty Oxford (power-isl)
13:50	Interlayer Metals for Zero-Excess Li Metal Batteries: A Multiscale Approach Combining Machine Learning Potentials and DFT		Neubi Xavier Jr. Surrey (power-cai)
14:10	**Invited:** BioSimDB: Data Tools and Infrastructure for Biomolecular Simulation		James Gebbie PSDI, STFC
14:50	PSDI Thematic Portals		Abraham Nieva de la Hidalga, Cardiff
15:10	REMatch plus SOS: Machine-learning-accelerated structure prediction for supported metal nanoclusters		Yunyu Zhang UCL(discov-cat)
15:30	**Tea**		
Session 2:	Surfaces and Interfaces	**Chair** TBA	
16:00	Modelling core-electron binding energies at metal oxide surfaces		Johannes Lischner Imperial (lis)
16:20	Modelling of fcc Ruthenium Surfaces and Particles with Hydrogen		Marietjie Ungerer Leeds (react-lee)
16:40	Exploring the possible superconducting mechanism of infinite-layer nickelates		Hangbo Qi UCL (bulk-sok)
17:00	Atomic-Scale Insights into Passivation and Halide Mixing in 3D and 2D Halide Perovskites		Vikram Oxford (nano-isl)
17:20	Atomistic modelling of SiO_2/Ta interfaces		Margherita Buraschi UCL (shl)
17:40	**Poster Session** Starting with 45s-lightning presentations (1 slide per poster) Session will include food and refreshments		
20:00	Session ends		

Tuesday 8th July			
Session 3:	Bulk	**Theme Leader** TBA	
9:00	**Invited:** Challenges and opportunities for Computer Modelling in calculating X-ray absorption Near Edge Structure (XANES) – a powerful tool for local structure determination		Gopinathan Sankar UCL
9:40	QM/MM simulations of intrinsic point defects in Sr based materials SrO and $SrTiO_3$		Taifeng Liu Henan (sok)
10:00	QM/MM Investigations of Defects in MgO and Their		Liam Morgan

	Use as a Model System for High-Tc Superconductivity		UCL (cat)
10:20	Computational prediction of $Cd_2Sb_2O_7$ as a candidate TCO		Peter Russell Birmingham (dos)
10:40	Investigating Electron Localisation in Defective Bulk Ceria with Dispersion Corrected DFT		Thomas Hill Cardiff (react-cat)
11:00	**Coffee**		

Session 4:	Reactivity	**Theme Leader** Umberto Terranova	
11:20	**Invited (New Investigator):** Computation for a green future: exploring the catalytic conversion of methane		Matthew Quesne Leeds (que)
12:00	Computational investigation of the Fe_xRh_y alloy structures and the mechanism and selectivity of CO_2 hydrogenation		Shihia Sun UCL (cat)
12:20	Developing Next-Generation Catalysts for Iso-butanol Production Using Machine Learning		K. Agrawal Cardiff (log)
12:40	Amide-Rich NaH as a Highly Active Catalyst for Ammonia Synthesis		Michael D. Higham UCL (cat)
13:00	**Lunch**		
Session 5:	Algorithms	**Chair** TBA	
14:00	Workflows for QM/MM Simulations of Metal Oxides		Oscar van Vuren Cardiff (log)
14:20	Hybrid QM/MM and Machine Learning for Zeolite Catalysts and Silica Polymorphism		Jamal Abdul Nasir UCL (react-sok)
14:40	First-principles modelling of infrared and Raman spectra		J. M. Skelton Manchester (ske)
15:00	The Crystal Isometry Principle infers chemistry from geometry		Vitaliy A. Kurlin Liverpool (dar)
15:20	**Invited:** TBA		Mark Storr AWE
16:00	**Coffee**		
Session 6:	Kostya Trachenko	**Chair** Richard Catlow	
16:30	Radiation damage: from glasses through solid oxides/ceramics to metals.		Ilian Todorov STFC
16:50	The effect of impurities and irradiation on the glass network – Cs_2O-loaded iron phosphate case study		Cillian Cockrell Bangor (enviro-kos)
17:10	Calculating system properties on-the-fly in DL_POLY 5		H. L. Devereux QMUL (algor-kos)
17:30	TBA		TBA
18:00	session ends		
19:00 – 22:00	**Conference BBQ Dinner**		Daresbury Caterers

Wednesday 9th July			
Session 7:	Bio and Soft Matter	**Chair** Jamieson Christie	
9:00	Nanoscale Non-adiabatic Dynamics Simulation of Charge Generation in Organic Solar Cells		Filip Ivanovic UCL (biosoft-blu)
9:20	Investigating the conductivity of Multi-Heme Cytochromes		A.M. Petho UCL (biosoft-blu)
9:40	Elucidating the effect of doping on the mechanical and chemical stability of hydroxyapatite		Mahdi Tavakol Oxford (biosoft-tan)
10:00	**Coffee**		
Session 8:	Excalibur	**Chair** Scott Woodley	
11:00	**Invited:** Integrating quantum computing with HPC		Viv Kendon Strathclyde
11:40	TBA		Bruno Camino UCL
12:00	TBA		Rajany KV STFC
12:20	Porting ONETEP and CASINO onto GPUs		Ben Thorpe York
12:40	CASINO		Neil Drummond Lancaster
13:00	**Lunch**		
	Reactivity / Bulk	**Chair** David Willock	
14:10	Au and Au_3Cu nanoclusters as catalysts for light-driven CO oxidation		Igor Kowalec Cardiff (react-cat)
14:30	Investigating Hydrogen Interaction with Defective and Doped MgB_2 via Density Functional Theory		Navaratnarajah Kuganathan Nottingham (bulk-lin)
14:50	DFT & Data Mining Assisted Catalyst Discovery of Cu-based Alloys for CO2 Hydrogenation to Alcohols		Z. Lu Cardiff (react-log)
15:10	Localised electron states in Amorphous Alumina		Jack Strand UCL (bulk-shl)
15:30	**MCC General Meeting**		
16:30	Close		

1st reserve	Mechanism of CO_2 Reduction to Methanol with H_2 on an Iron(II)-scorpionate Catalys	Chengxu Zhu Manc'ter (react-que)

Summary of Poster Presentations

1	Design and development of novel composite electrodes for high-energy density supercapacitors	Abeer A. Hdadai Newcastle (power-jad)
2	A Computational Study of CO2 Methanation over Low-index Nickel Surfaces	M. Alotaibi UCL (react-cat)
3	Catalytic Partial Oxidation of Methane using an Yttria-Stabilized Zirconia Catalyst	Erze Gao UCL (react-cat)
4	Investigation of Li-N-H phase space for next generation Li-ion electrolytes	Peter J. Graham Birmingham (power-dos)
5	Computational Modelling of Zeolite-Catalysed DMN Synthesis	Oliver Morris Cardiff (react-cat)
6	Data-driven design of electroactive metal-organic frameworks	Ashna Jose Imperial (discov-wal)
7	Promoting MgH_2 Destabilization Through Reactive Elemental Additives	Navaratnarajah Kuganathan Nottingham (bulk-lin)
8	Germanium Dioxide – A UWBG Material for Optoelectronic Applications	Jacob C. Baggott Birmingham (bulk-dos)
9	A Computational and Theoretical Study on Methanol Synthesis	Matis Ferrini Lincoln (react-arc)
10	Understanding Polarisation at Ferroelectric-perovskite Interface – A molecular Dynamic Perspective	Tingwei Li QMUL (surfin-but)
11	First-principles study of the thermoelectric properties of $Sn(S_{1-x}Se_x)$ alloys	Min Zhang Manchester (power-ske)
12	Structural Characterisation and Analysis of $NaTaO_xC_{l6-2x}$ for Solid¬—state Sodium Batteries	Abigail C. Parsons Birmingham (power-dos)
13	Effect of Nitrogen Incorporation in a-HfO_2	Isaac Mackley UCL (bulk-shl)
14	Vibrational Dynamics and Mechanical Anisotropy in Open Framework Materials: Computational Design Rules for MOF-based Triboelectric Generators	Debayan Mondal Oxford (discov-tan)
15	Carbon Nitride-Supported Metals for the Selective Oxidation of HMF to DFF	Xue Yong Liverpool (react-)
16	Mg Doping in GaN: application of the MACE Potentials	Yuxi Zhang UCL (bulk-smw)
17	Al Doping in ZnO: application of the MACE Potentials	Zhuoran Ji UCL (bulk-smw)
18	Modelling the phase transition of VO_2	Zichao Wang UCL (buk-smw)
19	Quantum Inspired Optimisation of $LiMnO_2$	Selin Kilic UCL (algor-smw)