MCC 5th Conference - Programme

Wednesday 28th June			
12:30	**Registration Desk Open**		**Daresbury Laboratory**
12:30	**Lunch**		
Session 1:	Low Dimensional Materials	**Chair** Umberto Terranova	
13:45	**Start – Welcome Address**		
13:50	**Invited:** Disorder?		Neil Allan Bristol
14:20	Predicting the Atomic Structures of Nanoclusters for Compounds with 1:3 Stoichiometry		Dong-Gi Kang UCL (smw)
14:40	Multiscale modelling of the electrical conductivity of carbon nanotube films		Thomas R Durrant UCL (shl)
15:00	**Invited:** ONETEP, with some exemplar applications thrown in.		Chris Skylaris Southampton
15:30	**Tea**		
Session 2:	Reactivity	**Theme Leader** David Willock	
16:10	**Invited:** Current Challenges in Catalytic Science		G Hutchings Cardiff
16:50	Mechanism of NH_3 Synthesis on Fe_3Mo_3N		M. D. Higham UCL (cat)
17:10	The Electronic Structure and Catalytic Activity of a Ru3 Cluster Embedded on Nitrogen-doped Graphene		Yao Zhao Oxford (mcg)
17:30	Computational investigation of NiOOH, from bulk to catalysis		Ruotao Yang UCL (cat)
17:50	**Poster Session** Starting with 24 45s-lightning presentations (1 slide / poster)		
20:00	Session ends		

Thursday 29th June			
Session 3:	Bulk	**Chair** Chris Lorenz	
9:10	**Invited:** Amorphous ZnO: Structure, Stability and Charge Trapping		David Mora-Fonz HTU, Mexico
9:40	Ab-Initio Molecular Dynamics Simulations of Substoichiometric Amorphous Alumina		Jack Strand UCL (shl)
10:00	Unravelling Hydrogen Bonding Behaviours and their Impact on Proton Conductivity in Supramolecular Cages		Lei Lei Nottingham (lin)
10:20	Investigation of unintentional aggregation of impurity-related defects within 4H-SiC		N. Smith UCL (shl)
10:40	Simulation of correlation driven metal-insulator transitions in real solids using deep neural networks		H. Sutterud Imperial (fou)
11:00	**Coffee**		

Session 4:	Surfaces and Interfaces	**Theme Leader** Matthew Watkins	
11:30	The effect of ceria surface composition on scavenging reactive oxygen species		Khoa Minh Ta Huddersfield (mol)
11:50	Modelling the effect of H in the formation, stabilisation and evolution of voids in polycrystalline Cu		Vasileios Fotopoulos UCL (shl)
12:10	Simulating Hydrogenation in Magnesium Through the Application of Machine Learning Models		Oliver M. Morrison Nottingham (lin)
12:30	Study of Hydroxyl Nests in Zeolites		Alec Desmoutier UCL (cat)
12:50	**Lunch**		
Session 5:	Power	**Theme Leader** Lucy Whalley	
13:50	Bulk and Surface Contributions to Ionisation Potentials of Metal Oxides		Xingfan Zhang UCL (sok)
14:10	Bismuth oxychalcogenide materials for thermoelectric applications		Joseph M. Flitcroft Manchester (ske)
14:30	Relating the formation energies for oxygen vacancies defects to the structural properties of tungsten oxides		R Kerr Lancaster (mur)
14:50	Controlling the heat transport in thermoelectric materials		Jonathan M. Skelton Manchester (ske)
15:10	**Coffee**		
Session 6:	Environment and Algorithms	**Chair** Scott Woodley	
15:40	**Invited:** The Baskerville Tier-2 Service		Jon Wakelin Birmingham
16:00	**Invited:** The GW4 Tier-2 Service		Steven Chapman Bristol
16:30	Oxygen-functionalised graphene: structure, properties, and potential for phosphate sensing		Natalia Martsinovich Sheffield (enviro-nat)
16:50	An Efficient Model for sp-Lone Pair Cations		Woongkyu Jee UCL (algor-smw)
17:10	**Invited:** Fundamental Principles of a Virtual Tokamak Fusion Reactor		Sergei L. Dudarev UKAEA
17:40	session ends		
18:00 – 21:00	**Conference BBQ**		

Friday 30th June			
Session 7:	Materials Discovery	**Chair** Marco Molinari	
9:00	Optimisation of decision sequences from selection of elements to chemical formulae of functional materials		A. Vasylenko Liverpool (dar)
9:20	Computational Modelling of Wide Band Gap Transparent Conducting Oxide Sb_2O_5		Ke Li UCL (dos)
9:40	A computational study characterising the intrinsic and extrinsic doping profile of ZnS		S. Aggarwal UCL (dos)
10:00	Organosulfide-Halide Perovskites incorporating Zwitterions		Santanu Saha Oxford (fil)
10:20	**Coffee**		
Session 8a:	Biomaterials and Soft Matter	**Chair** Richard Catlow	
10:50	**Invited:** Prediction of critical micelle concentrations in surfactant mixtures by DPD simulations		Guadalupe Jiménez-Serratos, STFC
11:20	Structural and dynamic properties of poly(styrene-co-maleic anhydride) at the interface of conjugated polymers		Christian D. Lorenz KCL (lor)
11:40	Iron-sulfur peptides for an efficient electron transfer to the hydrogenase enzyme		Umberto Terranova Buckingham (react-ter)
Session 8b:	MCC General Meeting		
12:00	computa1onal simula1ons to understand molecular crystals and crystallisa1on - New Member Code acc		Aurora Cruz-Cabeza Durham
12:20	Generating a Machine-Learned Equation of State for Fluid Properties - New Member Code mul		Erich Muller Imperial College
12:40	ARCHER2 update		William Lucas EPCC
12:50	YOUNG update		Heather Kelly UCL

13:00	Lunch	
14:00	MCC Main Meeting	
16:30	Close	

Reserve Talk	How bulk and surface properties of X_4SiC_3 (X=Ti,V,Nb,Zr) tune reactivity: A computational study	Matthew Quesne Cardiff (react-cat)