MCC 6th Conference - Programme

Wednesday 3rd July			
11:30	**Registration Desk Open**		**Daresbury Laboratory**
12:00	**Lunch**		
Session 1:	Excalibur (PAX-HPC)	**PI** Scott Woodley	
13:30	Acceleration of Electronic Structure Codes on Heterogeneous Hardware		Marcello Puligheddu STFC (Hartree)
13:50	Towards Exascale Smoothed Particle Hydrodynamics on Heterogeneous Supercomputers		Abouzied Nasar Manchester
14:10	CASTEP API and GPU parallel optimisation		TBA York
14:30	SWIFT2 – Task based parallelism		Mladen Ivkovic Durham
14:50	**Invited:** Accelerate Time-To-Science using the NVIDIA platform		Filippo Spiga Nvidia
15:30	**Tea**		
Session 2:	Surfaces and Interfaces	**Chair** Lucy Whalley	
16:00	Atomistic Modeling of the Isotopic Enrichment via Ion Irradiation of Silicon-28 Layers for Quantum Architectures		Samuel Murphy Lancaster (mur)
16:20	The CAT and SOD nanozymatic activities of nanoceria		Khoa Minh Ta Huddersfield (mol)
16:40	Polarization control in nanoscale ferroelectrics		Chiara Gattinoni KCL (gat)
17:00	Polymeric nanoparticle strategy for improving passivation and stability of perovskite solar cells: insights from DFT and AIMD simulations		Lei Zhu Oxford (isl)
17:20	Development of ReaxFF potential for phosphate-based bioglasses		Jamie Christie Loughborough (jam)
17:40	**Poster Session** Starting with 30s-lightning presentations (1 slide per poster) Session will include food and refreshments		
20:00	Session ends		

Tuesday 4th July			
Session 3:	Bulk	**Theme Leader** Alex Shluger	
9:00	**Invited:** Capturing Complex Semiconductors from First Principles		Volker Blum Duke University
9:40	Role of Lithium Entropy in the Polymorphism of Ion Conductor Li_3PS_4		Andrey Poletayev Oxford (isl)
10:00	Ab Initio Design of Molecular Qubits with Electric Field Control		William Morrillo Manchester (chi)
10:20	Polaron Induced Degradation of a-Ta_2O_5 ReRAM		Teo Cobos

	devices for Neuromorphic Computing		UCL (shl)
10:40	Accurate and Efficient Spin–Phonon Coupling and Spin Dynamics Calculations for Molecular Solids		Nicolas Chilton Manchester (chi)
11:00	**Coffee**		

Session 4:	Reactivity	**Theme Leader** David Willock	
11:20	Selective Catalytic Reduction of Nitrogen Oxides with Ammonia over Cu-CHA and Fe-BEA Zeolite		Jamal Abdul Nasir UCL (sok)
11:40	Computational Insights into the Stability and Phase Transition of Cobalt Oxide Nanoparticles for Fischer-Tropsch Catalysis		Akash Hiregange Cardiff (log)
12:00	Mechanism of photocatalytic water splitting on the pristine $CuWO_4$ (010) surface		Xuan Chu Leeds (lee)
12:20	Multiscale investigation of the mechanism and selectivity of CO_2 hydrogenation over Rh (111)		Shihia Sun UCL (cat)
12:40	Single-atom catalysis for carbon dioxide dissociation using greigite-supported M_1/Fe_3S_4(111) (M = Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn) under electrostatic fields		David Santos Carballal Leeds (lee)
13:00	**Lunch**		
Session 5:	Algorithms	**Chair** Richard Catlow	
13:50	**Invited:** Machine learning and beyond DFT methods: quantitative materials modeling at your fingertips		Georg Kresse University of Vienna
14:30	Machine learning the DFT+U projectors to model polarons in energy materials		Amit Chaudhari Cardiff (log)
14:50	Machine Learning Optimisation and Structural Dynamics of Hybrid Halide Perovskites		Xia Liang Imperial (wal)
15:10	Developing Standardised Modelling Workflows for QM/MM Simulations of Metal Oxides		Oscar van Vuren Cardiff (log)
15:30	**Coffee**		
Session 6:	Celebrating 30 years!	**Chair** Scott Woodley	
16:25	Overview and History		Scott Woodley
16:45	Talks from the first MCC investigators – what we proposed 30 years ago and today!		Richard Catlow
17:00			Rob Jackson
17:15			Steve Parker
17:30			Kenneth Harris
17:45			John Harding
18:00	session ends		
19:00 – 22:00	**Conference BBQ Dinner**		Daresbury Caterers

Friday 5th July			
Session 7:	Biosoft & Discov	**Chair** Chris Lorenz	
9:00	RAFFLE: Structure prediction for material interfaces		Ned Taylor Exeter (discov-hep)
9:20	Data distribution aware models for high throughput materials discovery		Lei Lei Nottingham (lin)
9:40	Unbiased Monte-Carlo Approach to Study Discharging of a Cathode		Woongkyu Jee UCL (smw)
10:00	**Invited:** Utilisation of ionic liquids and catalysis for net zero applications		Chris Hardacre Manchester
10:40	**Coffee**		
Session 8:	Power	**Chair** Umberto Terranova	
11:20	Automated Strategies for Potential Development: Investigating Tetrahedrite Diffusion		Andrew Duff STFC (pan)
11:40	Unforeseen Phononic Crystal In Li Electrodes		Harry Mclean Exeter (hep)
12:00	Temperature-dependent dynamic disproportionation in $LiNiO_2$		Andrey Poletayev Oxford (isl)
12:20	Ab initio workflow for predicting the figure of merit of thermoelectric materials		Jonathan Skelton, Manchester (ske)
12:40	**Lunch**		
	Surfaces and Interfaces	**Chair** Marco Molinari	
14:00	Unusual properties: A study of oxide interfaces		Ned Taylor Exeter (hep)
14:20	Radiation damage in $YBa_2Cu_3O_7$ high-temperature superconductors: an ab initio molecular dynamics study		Ashley Dickson Lancaster (mur)
14:40	Understanding the structural and electronic properties of a complex defect-bearing heteroepitaxial binary copper oxides interface		Aleksandar Živković Kiel University (lee)
15:00	Variable Band Edge Positions in Metal Oxides: Bulk, Surface, and Environmental Effects		Xingfan Zhang UCL (sok)
15:20	**MCC General Meeting**		
16:45	Close		

Standby Talk	Exploring formate adsorption on diluted Cu alloys	Zhongwei Lu Cardiff (log)
Standby Talk	Modelling of magnetochiral dichroism for lanthanide (III) complex	Maxime Grasser Manchester (chi)
Standby Talk	Thermal transport in TMDC heterostructures	Francis Davies Exeter (hep)