MCC 8th Conference - Programme

Wednesday 1st July			
11:30	**Registration Desk Open**		**Daresbury Laboratory**
12:00	**Lunch**		
Session 1:	Algorithms	**Chair** TBA	
13:10	ML-PEG: machine learning performance and extrapolation guide		Elliott Kasoar STFC (COSEC)
13:30	Machine-learned potentials for silica polymorphism and MgO defect chemistry		Jamal Abdul Nasir UCL (smw)
13:50	**Invited:** Simulating molecules and materials on an ion trap quantum computer		David Munoz Ramo Quantinuum
14:30	AI for clusters: extracting structural data from images through deep learning		Cyril Xu UCL (smw)
14:50	MolSim++: GPU confined particle dynamics project		Joseph Thacker STFC (COSEC)
15:10	PATINA: A modular software approach towards composable & reproducible computational materials workflows		Gokay Avci UCL (smw)
15:30	**Tea**		
Session 2:	Discovery	**Chair** TBA	
16:00	A multi-scale mixture of experts model for cross-size structural prediction of Cu nanoparticles		Yunyu Zhang UCL (cat)
16:20	Integrating ML and AI with classical simulations for automating materials discovery		Chris Collins Liverpool (dar)
16:40	FAIR-MOFs: Structure-centred synthesis inference from three-dimensional structures of metal-organic frameworks		Dinga Wonanke NTU (add)
17:00	DeepHydride: A machine-learned interatomic potential based framework for high-throughput discovery of metal hydrides		Lei Lei Nottingham (lin)
17:20	The morphology of sub-nanometer clusters on surfaces		Thomas Hill Cardiff (cat)
17:40	**Poster Session** Starting with 30s-lightning presentations (1 slide per poster) Session will include food and refreshments		
20:00	Session ends		

Thursday 2nd July			
Session 3:	Bulk	**Chair/Theme Leader** Keith McKenna	
9:00	**Invited:** Equations to Enterprise: Turning Computational Materials Research into Industrial Impact		David Gao Nanolayers
9:40	The solid-state chemistry of thorium-229 nuclear clocks		Harry Morgan Manchester (hwt)

10:00	Computational discovery of symmetry-protected and distortion-induced topological phonons in half-Heusler alloys	Sam Ginzburg Cambridge (sjj)
10:20	Cage electron mediated hydride formation in Mayenite electride	Navaratnarajah Kuganathan Nottingham (lin)
10:40	QM/MM investigations of defects in MgO and La_2CuO_4 and other related materials	Liam Morgan UCL (sok)
11:00	**Coffee**	

Session 4:	Surfaces and Interfaces	**Theme Leader** TBA	
11:20	**Invited:** CRYSTAL, an ongoing project for a chemical approach to solids		Silvia Maria Casassa University of Torino
12:00	Phonon and thermal transport effects of extended defects in reduced γ-WO_3 via machine learned interatomic potentials		Anas Siddiqui York (mck)
12:15	Towards modelling vibration-assisted hot-carrier processes in metallic nanoparticles		Damian Contant KCL (iva)
12:30	Oxygen scavenging at a SiO_2/Ta interface: a first-principles study		Margherita Buraschi UCL (shl)
12:45	Oxygen-driven evolution of novel $\Sigma5$ tilt boundaries in Anatase TiO_2 by in-situ eSTEM/TEM		Jack Fawcett-Hough-ton, York (mck)
13:00	**Lunch**		
Session 5:	Reactivity	**Chair/Theme Leader** Richard Catlow	
14:00	**Invited:** TBA		Guillaume Maurin Montpellier II
14:40	Effects of surface nanostructure of metal co-catalysts for photocatalytic conversion of methane: a theoretical study		Natalia Martsinovich Sheffield (nat)
14:55	Impact of the presence of Au on activity and selectivity of Cu/ZnO catalysts for methanol synthesis		Michael D. Higham Cardiff (cat)
15:10	Nitrogen evolution reaction study on Ru supported clusters and Ru(0001) surface		A. Amanzhol Cardiff (rol)
15:25	Investigating the formate pathway for CO_2 to MeOH over Pd/ZnO catalysts		E. McCarthy Cardiff (wil)
15:40	**Coffee**		
Session 6:	Power	**Chair** TBA	
16:10	**Invited:** Chemo-mechanics and Kinetics of Li_xNiO_2 - unravelling hidden complexities		Karsten Albe TU Darmstadt
16:50	Vibrational spectra of zirconolite		Joseph Flitcroft Manchester (bulk-ske)
17:05	Correlation of polarons and highly charged interstitials in metal oxides		Isaac Mackley UCL (bulk-shl)
17:20	Multiscale modelling of grain boundaries and extended defects in halide perovskites using machine-learning potentials and DFTB		Junke Jiang York (power-mck)

17:35	The Monte Carlo threshold algorithm in crystal structure prediction: introducing intramolecular degrees of freedom		Pedro Juan-Royo Southampton (discov-day)
17:50	session ends		
18:00 – 21:00	**Conference BBQ Dinner**		Daresbury Caterers

Friday 3rd July			
Session 7:	Reactivity	**Chair/Them Leader** David Willock	
9:00	Rational design of sulphur-terminated MXenes for efficient CO_2 conversion into carbon neutral methanol production		Moses Abraham Leeds (lee)
9:20	The pressure-dependent surface state of cobalt during Fischer-Tropsch synthesis		Jack Swallow Manchester (swa)
9:40	Single- and dual-atom catalysts for the CO_2 reduction reaction		L. Rivera-Blair Cardiff (rol)
9:55	Updates to phonopy-spectroscopy: first-principles modelling of infrared and Raman spectra		J. Skelton, Manchester (bulk-ske)
10:15	Field-free coexistence of skyrmions and anti-skyrmions induced by higher-order interactions and biaxial strain in the NiI_2 monolayer		Zebin Wu UCL (nano-sok)
10:30	**Coffee**		
Session 8:	Algorithms	**Chair** TBA	
11:00	**Invited:** From Lithium Batteries to Perovskite Solar Cells - Atomistic Insights into Energy Materials		Saiful Islam Oxford (isl)
11:40	Reliable and reproducible benchmarking of DFT codes on GPUs: A CASTEP case study		Oscar van Vuren Cardiff (log)
11:55	DL-FIND: Benchmarking methods for geometry optimisation		Thomas R. Durrant STFC (COSEC)
12:10	Implementing extendable workflows for QM-in-QM embedding		Gabriel Bramley Cardiff (log)
12:25	**Lunch**		
Session 9:	Enviro / Biosoft	**Chair** Umberto Terranova	
13:30	Machine learned potentials for Li based reactive hydride composites		Oliver Morrison, Nottingham (surfin-lin)
13:50	Effects Of Isomerism on Porous framework materials: Window Edition – How Does Isomerism Affect A Guest Molecules Ability To Enter A Pore		Saad Choudry NTU (discov-add)
14:05	Probing nuclear extremes in lithium ceramics: multiscale simulations with machine-learnt interatomic potentials		Cillian Cockrell Bangor (enviro-cil)
14:25	Molecular architecture and oligomerisation as determinants of micelle structure		Chris Lorenz KCL (biosoft-lor)
14:45	Close		

15:00	**MCC Meeting of Group Leaders** The future of the MCC: open discussion		
16:45	Close		

Summary of Poster Presentations

1	A Density Functional Theory study on the Point defects in PuO_2	Paris-Rose Dawson Huddersfield (bulk-mol)
2	Atomistic Simulation of Liquid Electrolytes on Argyrodite Surfaces for Hybrid Solid-Liquid Lithium Batteries	Felix Scott Newcastle (surfin-jad)
3	Using DFT Simulations to Investigate Ammonia Conversion to Hydrogen on Transition-Metal Based Catalysts	Sebastian Teodorescu-Oros, Surrey (react-cai)
4	Computational Modelling of Photocatalytic Conversion of Organic Molecules into Biofuel	Luke Andrew Sheffield (react-nat)
5	Computational Study of Sodium-Ion Migration and Defect Chemistry in Na_8SnP_4-Based Solid Electrolytes	Patabandi Mudiyanselage Birmingham (power-dos)
6	Exploring the Defect Chemistry of Potassium Tantalate	Urvi A. Joshi Birmingham (bulk-dos)
7	A Computational and Experimental Study of the Methanol Synthesis catalyst	Matis Ferrini Lincoln (react-arc)
8	Amorphous-like Thermal Conductivity and High Thermoelectric Figure of Merit in "π" SnS and SnSe	Min. Zhang Manchester (power-ske)
9	Investigating Vacancy Defects in a Candidate Transparent Conducting Oxide, $LaSb_3O_9$	Jack N. Beattie Birmingham (bulk-dos)
10	Pressure Driven Evolution of Various Metal Hexaborides	Abubakar Imran Manchester (bulk-hwt)
11	First-Principles Investigation of Band Alignment and Defect-Induced Electronic States at 2D–3D Perovskite Interface	Shaojun Hao Newcastle (surfin-jad)
12	Computational Study of Thorium-Containing Host Materials for use in Thorium-229 Nuclear Clocks	Dewi Parry Manchester (bulk-hwt)
13	Benchmarking the Energy Ranking of Molecular Crystals at the Meta-GGA Level	Namrata Ramesh Leeds (bulk-arp)
14	Computational Investigation of CO_2 Methanation over Ni and Ni-Alloy Catalysts	M. Alotaibi UCL (react-cat)
15	Periodic DFT Investigation of CO_2 Hydrogenation on Clean and Fe-Doped Ni(111) Surfaces	Linqing Dong UCL (react-cat)
16	A Study of H_2O-Promoted CO_2 Coupling to Ethanol on the Cu(100) Surface	Zhenze Zhao, UCL (react-cat)
17	Modelling Charge Carriers in Cuprate High-Temperature Superconductors	Taochun Ma UCL (bulk-sok)
18	QM/MM Calculations for ZnO (10-10) and the CO_2 Adsorption	Shumin Li Cardiff (react-wil)
19	Modelling Excited States of MOFs NU-1000 and NU-901 Using Cluster and Periodic Approaches	Selin Kilic UCL (discov-rco)
20	Machine-Learned Structure Prediction of TiO_2 Clusters Using Fine-Tuned MACE Potentials	Anna-Lena Singer UCL (nano-smw)
21	Machine Learning Study of Charge Compensation Mechanisms in Zr-Doped ZnO at low doping Concentration	Yulin Song UCL (power-smw)
22	Spin-Polarised DFT Study of Antiperovskite Materials for Lithium-Ion Battery Applications	Ruojie Huang UCL (power-smw)
23	Sampling Defect Complexes in Beryllium Doped GaN Using a Machine Learning Interatomic Potential	Yuxuan Liao UCL (power-smw)
24	Model Collapse under Iterative Self-Training of Generative Models	Joley Yuhui Lin UCL (discov-but)
25	Atomistic Modelling of CoO_x/TiO_2 interfaces: Elucidating Metal-Support Interactions in Fischer-Tropsch catalysts	Akash Hiregange Cardiff (surfin-log)

26	Time-Resolved Simulation of Shock-Driven Energy Redistribution in Crystalline Energetic Materials	Mateusz Mojsak Birmingham (bulk-adm)
27	Mechanochemically Promoted CO_2 Methanation over Co-CeO_2 Catalysts via Collision-Induced Charge Effects	Weiwei Xu Liverpool (react-xue)