12:30	**Registration Desk Open**		**Daresbury Laboratory**
12:30	**Lunch**	**14:00 Start – Welcome Address**	
Session 1:	Biomaterials & Soft Matter	**Theme Leaders** J Christie, C Lorenz	
14:05	**Invited**: TBA		Sarah Harris CCPBioSim, Leeds
14:35	Temperature Dependence of Charge Mobility in Rubrene from Fragment Orbital-Based Surface Hopping		**Jan Elsner** UCL (blu)
14:55	Effect of polymer topology on the self-assembly of micelles		Chris Lorenz KCL (lor)
15:15	Overview of CoSeC support for MCC		Tom Keal CoSeC
15:35	**Tea**		
Session 2:	Environment & Smart Mater.	**Theme Leaders** J Harding, N Harrison	
16:00	**Invited:** From Gomberg to graphene and beyond: new multifunctional 2D materials based on persistent radicals		Stefan Bromley Barcelona
16:30	Thermodynamics up to the melting point in a TaVCrW high entropy alloy: Systematic ab initio study aided by machine learning potentials		Ying Zhou Loughborough (bulk-pan)
16:50	Thermal conductivity of radiation damaged tritium breeder materials		Megha Sanjeev Lancaster (mur)
17:10	An *ab initio* investigation of the impact of intrinsic defects on the thermal properties of CeO_2		Thomas Smith Huddersfield (bulk-mol)
17:30	**Poster Session** Starting with lightning presentations (1 slide per poster)		
20:00	Session ends		

Thursday 7th July			
Session 3:	Fund. of Low Dim. Materials	**Theme Leaders** M Molinari, S Woodley	
9:10	**Invited:** Predicting structure formation and trans-formation in low-dimensional systems via studying their energy landscapes		Christian Schön MPI, Stuttgart
9:40	BN doped PAHs – Towards 2D molecular recognition		Jack Warren Cardiff (rol)
10:00	Chlorine Activated Stacking Fault Removal Mechanism in thin Film CdTe Solar Cells: the missing Piece		Pooja Goddard Loughborough (pan)
10:20	Understanding nucleation of Co and Mn nanoclusters on anatase (101) surface		Pavel Stishenko Cardiff (log)
10:40	Chiral valley phonons and flat phonon bands in moiré materials		Indrajit Maity Imperial (lis)
11:00	**Coffee**		

Session 4:	Fund of Surfaces &Interfaces	**Theme Leader** B Slater, M Watkins	
11:20	Phosphate adsorption on {111}, {110}, and {100} surfaces of ceria: A DFT study		Khoa Minh Ta Huddersfield (mol)
11:40	The thermoelectric properties of Polyaniline-$SrTiO_3$ composites		Nathan Wood Huddersfield (mol/coo)
12:00	Obtaining Interfacial Free Energies from Atomistic Simulations using an Einstein Crystal Reference State		John Harding Sheffield (har)
12:20	Towards Modelling Realistic $WS_2/H_2O/SiO_2$ Interfaces		**Katherine Milton** UCL (shl)
12:40	**Lunch**		
Session 5:	Fund. of Bulk Materials	**Theme Leaders** A Shluger, K McKenna	
13:50	Approximating Many-Electron Wave Functions using Neural Networks		Matthew Foulkes Imperial (fou)
14:10	Anharmonicity and entropic stabilisation in zirconia from first principles		Kasper Tolborg Imperial (wal)
14:30	Exploring the Nanoparticle Exsolution Process in Perovskite Oxide		Ji Wu/ Steve Parker Bath (par)
14:50	The Impact of E Field on Defect Generation and Migration Processes in Dielectrics		Jack Strand UCL (shl)
15:10	**Coffee**		
Session 6:	Materials Discovery	**Theme Leaders** G Day, K Jelfs	
15:50	**Invited:** Computational Chemistry: An Industrial Perspective		Misbah Sarwar Johnson Matthey
16:20	Investigating the structure and stability of PdZn bi-metallic alloys by coupling density functional theory and cluster expansions		Lara Kabalan Cardiff (log)
16:40	Computational design of green ternary semiconductors for optoelectronic applications		**Santanu Saha** Oxford (fil)
17:00	Crystal structure predictions of organic halide salts		Joseph Glover Southampton (day)
17:20	**Invited:** Quantum computing for strongly correlated materials (QC-CCP, QEVEC)		François Jamet National Physical Laboratory
17:50	session ends		
18:00 – 21:00	**Conference BBQ**		

Friday 8th July			
Session 7:	Reactivity & Catalysis	**Theme Leader** D Willock, R Catlow	
9:10	Ab initio study of the Para-xylene Oxidation Redox Cascade		H Thomas Cardiff (log)
9:30	Interatomic-potential-based Computational Approaches for Modelling Defect Chemistry and Surface Oxidation of Solid Materials		Xingfan Zhang UCL (sok)
9:50	A mechanism for the CO_2-to-CO conversion catalysed by carbon monoxide dehydrogenase		**Umberto Terranova** Buckingham (ter)
10:10	Localised thermal levering events drive spontaneous kinetic oscillations in catalysis		Matt Quesne Cardiff (cat)
10:30	Coffee		
Session 8:	Energy Gen, Storage & Trans	**Theme Leaders** S Islam, A Walsh	
11:00	**Invited:** Exploring Battery Materials with Atomistic Simulations: Electrodes, Electrolytes, and Interfaces Thereof		René Windiks Materials Design
11:30	The Wadsley-Roth Materials Family as Functional Energy Materials		Adrien Richard UCL (cor)
11:50	Molecular Dynamics Simulations of Radiation Damage in High Temperature Superconductors		**S Murphy** Lancaster (mur)
12:10	Surprising improvement of SnS_2 properties through superlattice formation for battery applications		Conor Price Exeter (hep)
12:30	Intrinsic Defect Study on High-voltage Spinel $LiMn_{1.5}Ni_{0.5}O_4$ as Cathode Material for Li-ion Batteries		Jiayi Cen UCL (dos)
12:50	Final Remarks and Close		

Standby Talk	The hydrogen and water interactions with the pristine surfaces of monoclinic and orthorhombic $FeNbO_4$	Xingyu Wang Leeds (lee)