4th March

Time		Talk	Author	Title
09:30	10:30	Registration+ Refreshments		
10:30	10:35	Materials Chemisty Consortium (MCC)	Richard Catlow	MCC Welcome
10:35	10:40	Faraday Institution (FI)	Martin Freer	FI Welcome
10:40	11:10	Invited 1	Frank de Groot	Interpretation of X-ray Absorption Spectral Shapes
11:10	11:40	Organiser (FI)	Chris Skylaris	Large-Scale Atomistic Simulations of Battery Materials and Interfaces
11:40	12:20	Coffee		
12:20	12:50	Organiser (MCC)	Pooja Goddard	Materials Modelling of Nb based Oxides: Answering Battery Industry Relevant Research Questions
12:50	13:10	Contributed 1	Linquan Gong	Factors Governing Thermal Conductance Behaviour of Plasticized Single-Ion Conducting Polymer Electrolytes: A Molecular Perspective
13:10	13:30	Contributed 2	Vanessa K. Ward	A Rule that's Made to be Broken? Reframing the Arrhenius Law and the Calculation of Activation Energies for Ion Transport in Solid Electrolytes
13:30	14:30	Lunch		
14:30	15:00	Organiser (FI)	Martin Freer	Update on the Faraday Programme and UK-US Modelling Discussions
15:00	15:20	Contributed 3	Xue Yong	Beyond Funnel-like High Throughput Screening: An Expert Guided Multi-scale Nexus for Polynary Perovskite Electrocatalyst Exploration
15:20	15:40	Contributed 4	Navaratnarajah Kuganathan	Halide-Stabilised $LiBH_4$ as a Solid Electrolyte for Li-Ion Batteries
15:40	16:00	Contributed 5	Harry Mclean	Phonon Driven Non-equilibrium Triggers for Thermal Runaway in Battery Electrodes
16:00	16:30	Coffee		
16:30	17:00	Invited 2	Ieuan Seymour	Solid-state Paramagnetic NMR Calculations of Next-generation Battery Materials
17:00	17:20	Contributed 7	Jonathan M. Skelton	First-principles Modelling of Infrared and Raman spectra
17:20	17:40	Contributed 8	Matthias J. Golomb	Autonomous Data Engineering for Chemistry using general purpose models: A Case Study on Lithium Metal Electrolytes
17:40	18:00	Contributed 9	Neubi F. Xavier Jr.	Interface Design in Zero-excess Li Metal Batteries guided by DFT and Molecular Dynamics with Machine-Learning Interatomic Potentials
18:00		Close		
19:00	21:00	Dinner		

5th March

09:00		Day 2 open		
09:00	09:30	Invited 3	Robert Weatherup	Understanding Interfacial Reactions by Combining Operando Soft X-ray Spectroscopies with Spectral Simulations
09:30	10:00	Invited 4	James Dawson	Atomistic Understanding of Interfaces in Next-Generation Batteries
10:00	10:20	Contributed 10	Min Zhang	Amorphous-like Thermal Conductivity and High Thermoelectric Figure of Merit in "π" SnS and SnSe
10:20	10:50	Coffee		
10:50	11:20	Invited 5	Clotilde Cucinotta	From Constant-Potential Modelling to Sulfur-Engineered Hard Carbons: Ab-Initio Simulation of Electrochemical Interfaces
11:20	11:40	Contributed 11	Jyotsana Kala	Modeling Redox Potentials and Electrolyte-Organic Conjugated Polymer Interactions for Electrochemical Energy Storage Electrode Applications
11:40	12:00	Contributed 12	Simon A. Kondrat	Directly following Potassium Intercalation in Prussian Blue Cathodes via Potassium K-edge X-ray Absorption Spectroscopy
12:00	12:20	Contributed 13	Aswathy Girija	IoP Publishing
12:20	12:30	Organiser (MCC)	Scott Woodley	Charging/discharging MnO2: PAX-HPC (An excalibur funded project)
12:30	13:30	Lunch		
13:30	14:00	Invited 6	Emma Kendrick	Performance and Circularity in Sodium-Ion Batteries
14:00	14:20	Contributed 14	Beatrice Ricci	Investigating the Asymmetric Electrochemical, Structural and Electronic Properties of Mn-rich Li(Mn,Fe)PO4 Electrode Materials
14:20	14:40	Contributed 15	Richard Hennig	AI-Accelerated Screening of Electrolyte Solvents for High-Safety Batteries
14:40	15:00	Contributed 16	Qiong Cai	Modelling and Design of 3D Electrode Microstructures for Energy Storage Batteries
15:00	15:30	Coffee		
15:30	16:00	Invited 7	Alexander Squires	Modelling Structural Disorder and Ionic Transport in Sodium Oxychlorides
16:00	16:20	Contributed 17	Chris Davies	Modelling Fast Lithium-Ion Transport in the Argyrodite Solid Electrolytes
16:20	16:40	Contributed 18	Kit McColl	Predicting energy density retention in battery electrode materials using first-principles based modelling
16:40	17:00	Panel Discussion	Richard Catlow with Invited Speakers	Challenges in modelling energy application and battery materials
17:00		Close		