MECHANISTIC INSIGHTS INTO FAST ION CONDUCTION IN SOLID ELECTROLYTE AND CATHODE MATERIALS

Saiful Islam
Department of Chemistry, University of Bath, Bath BA2 7AY, UK

email address: m.s.islam@bath.ac.uk

Major advances in rechargeable lithium (or sodium) batteries require the discovery and characterisation of new materials. It is clear that a complete understanding of the properties of electrode and electrolyte materials for both Li- and Na-ion batteries requires fundamental knowledge of their underlying structural, ion diffusion and surface properties on the atomic- and nano-scales. In this context, advanced materials modelling [1] combined with structural and electrochemical techniques are now powerful tools for investigating these properties. This talk will highlight recent studies [2-4] in the following areas: (i) structural and mechanistic insights into fast lithium-ion conduction in Li$_4$SiO$_4$-Li$_3$PO$_4$ solid electrolytes; (ii) ion diffusion pathways in polyanionic cathode materials such as Li-sulfates (e.g. LiFeSO$_4$OH) and Na-phosphates (e.g. Na$_2$FePO$_4$F, Na$_4$M$_3$(PO$_4$)$_2$P$_2$O$_7$). The presentation will aim to demonstrate how the strong synergy of computer modelling and experiment has helped us to shed new light on the structure-property relationships of battery materials.

References