

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

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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_4SiO_4 - Li_3PO_4 solid electrolytes; (ii) ion diffusion pathways in polyanionic cathode materials such as Li-sulfates (e.g. LiFeSO_4OH) and Na-phosphates (e.g. $\text{Na}_2\text{FePO}_4\text{F}$, $\text{Na}_4\text{M}_3(\text{PO}_4)_2\text{P}_2\text{O}_7$). 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

- [1] M.S. Islam; C.A.J. Fisher, *Chem. Soc. Rev.*, 43, (2014) 185.
- [2] Y. Deng et al., *J. Amer. Chem. Soc.*, 137 (2015) 9136.
- [3] S.M. Wood et al., *J. Phys. Chem. C.*, 119 (2015) 15935.
- [4] C. Eames et al., *Chem. Mater.*, 26 (2014) 3672.