Mechanochemistry of Battery Materials at the Atomic-Scale

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The quest for improved energy storage to counter our dependence on fossil fuels and for the electrification of transport and large-scale storage is one of the greatest scientific challenges of the 21st century. This quest had led to the generation of considerable research interest in the discovery, design and development of materials for Li- and Na-ion batteries to enhance the safety and performance of current battery architectures. As an alternative to solvent-based processes and classic solid-state synthesis, the mechanochemical synthesis of cathode and solid electrolyte materials has received significant attention in recent years. In this presentation, I will describe the use of atomistic modelling methods, such as density functional theory and molecular dynamics, in exploring mechanochemical reactions and their effects on battery materials. In particular, I will present our recent work on the reaction between lithium metal and cobalt oxide in an effort to synthesise $LiCoO_2$ cathode materials, pressure effects and synthesis-property relationships in the Na_3PS_4 solid electrolyte and the ion transport properties of mechanochemically synthesised anti-perovskite solid electrolytes.

Biography

Dr. James A. Dawson is a Newcastle University Academic Track Fellow in the School of Natural and Environmental Sciences. His research utilises state-of-the-art computational techniques to investigate ion transport and defects in energy materials and their interfaces. Prior to joining Newcastle University, James held postdoctoral positions at the Universities of Bath and Cambridge, where he carried out simulations of battery materials with a particular focus on solid electrolytes for solid-state batteries. Following his PhD at the University of Sheffield working on perovskite materials for electronics, James spent two years at Kyoto University, Japan, as a JSPS Postdoctoral Fellow working on a variety of topics, including cathodes and electrolytes for battery and solid oxide fuel cell applications.