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PLENARY: Simulated synthesis, characterisation and performance of nano-architectured energy storage materials.

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Abstract content
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An increasing demand for energy and a shifting to renewable energy resources, has accelerated development of energy generation and storage for use in solar energy harvesting, electric vehicles, electricity grid backups. Enhanced performances of lithium ion rechargeable batteries, such as higher capacity, improved rate capability and sustained capacity retention for longer cycles are now achieved with various nano-architectures and were studied with a wide range of experimental techniques [1].

Electronic structure and atomistic simulations are capable of elucidating structural, transport and predicting performance of battery electrodes [2]. A major challenge associated with generating atomistic models is to capture the wealth of microstructural features observed experimentally and to follow evolvement of lithiated phases obtained after intercalation, associated with charging and discharging of batteries. One technique that is capable of spontaneously generating various nanostructures and introducing complex microstructures is the atomistic simulated amorphisation and crystallization method [3].

In this presentation such technique, which is based on molecular dynamics, used in conjunction with classical force fields, is employed to illustrate simulated synthesis and characterisation of different nano-architectures, i.e. nano- spheres, sheets, rods, porous and bulk of binary metal oxides such as MnO₂ and TiO₂. Furthermore, the nano-architectures are lithiated, to imitate charging and discharging, and their structural aspects and performance are characterized by simulated X-ray diffraction patterns and voltage profiles respectively. In particular, the relationship between mechanical properties, microstructural features and electrochemical activity in nanoporous and bulk structures is highlighted. Such connection is extended to why the ternary nano Li₂MnO₃, an end member of high voltage composite cathodes, is electrochemically active whilst its bulk form is inactive [4]. Lastly, nano-architectures, associated with the Li-Mn-O ternary were synthesised from amorphous spinel nanosphere. The resulting crystallised nano-architectures are characterised and the presence of a composite consisting of the layered Li₂MnO₃ and spinel LiMn₂O₄ together with a variety of defects, including grain boundaries and ion vacancies are observed, from XRDs and microstructural features. This is a step towards addressing the challenge of voltage fade in the composite layered spinel cathodes, which have high capacity and energy density [5]. Preliminary work beyond Li-ion batteries, particularly related to Li-S, will be introduced.

References

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