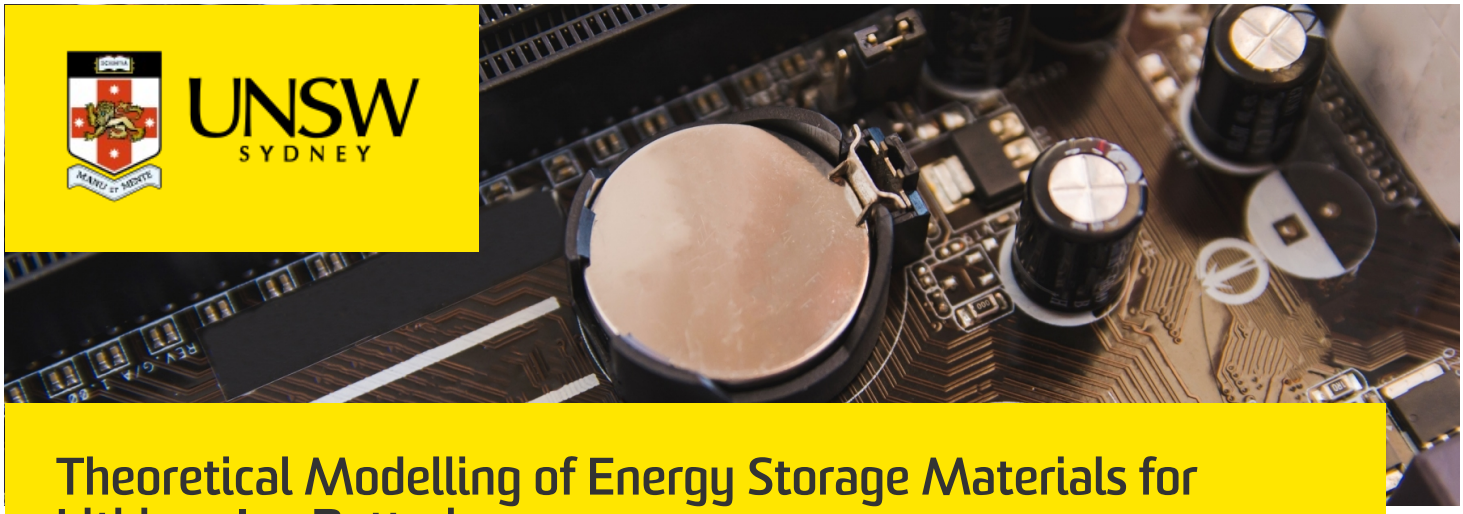

Theoretical Modelling of Energy Storage Materials for Lithium-Ion Batteries

Understanding how lithium-ion migrates during the electrode charge/discharge is important for improving the performance of lithium-ion batteries (LIB). Atomic simulation of the lithiation process provides the capability to recognise the mechanisms and key parameters, and use them to aid the design and manufacturing of LIB electrodes.

More Information

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Competitive advantage

- Knowledge in atomic simulation using density functional theory (DFT) and molecular dynamics (MD)
- Expertise in modelling the electrochemical interfaces
- Experience in modelling the defects in materials

Impact

- Demonstrated the electronic and ionic transports at the electrode/electrolyte interfaces
- Potential to develop a novel manufacturing (bottom-up) approach based on theoretical findings

Successful applications

- Identified lithiation mechanisms on a titanium dioxide electrode
- Identified important factors during lithiation process on a titanium dioxide electrode

Capabilities and facilities

- Quantum mechanics calculation such as VASP, CP2K and Gaussian
- Molecular mechanics calculation such as LAMMPS
- Computational electrochemistry and materials
- High performance computing cluster

Our partners

- Raijin National Computing Infrastructure
- Pawsey Supercomputing Centre