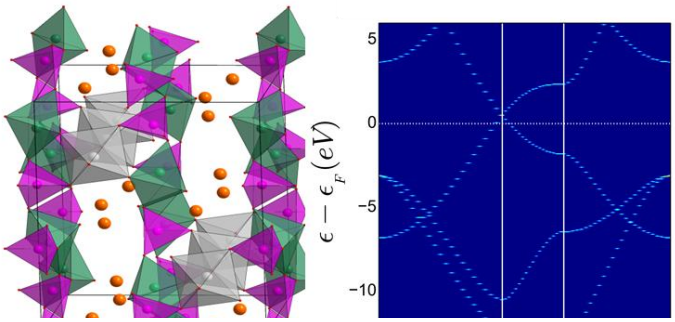
Project for Master Thesis at the Helmholtz Institute Ulm (HIU)/Ulm University

Computational Design of New Electrode Materials for Sodium-Ion Batteries

Dr. Holger Euchner

The intermittent, renewable resources like wind, solar and tidal energy require efficient and sustainable energy storage systems in balancing the power generation and demand. In addition, efficient electric energy storage is inevitable to power mobile electronic devices to next generation hybrid and electric vehicles. The efficacy of Li-ion batteries in energy storage is realized and initiated much effort in research to attain desirable properties like high specific energy, long cycle life/sustainability, safety and cost-effectiveness. Despite the improvements in the energy density and power density, problems still persist with Li-ion technology. Particularly with increasing energy requirements, there is a great demand for the technologies beyond Li-ion batteries (LIBs). In this context (specifically considering grid storage applications), sodium-ion batteries (SIBs) are evolving as low cost alternative to the state-of-the-art LIBs. Elementary properties of sodium, high abundance and low cost associated with sodium precursors made it a realistic alternative to lithium-ion chemistry. The energy density of sodium-ion batteries is comparable to state of the art LIBs. Furthermore, cost-effective, sustainable and safe battery systems can be built (top most priorities for grid application). Nevertheless, known candidates for insertion type electrode materials have been studied to a far lower extent. This offers a wide space for the investigation of compounds with unexplored compositions and properties, for the use in SIB applications.



Structure of a potential Na based cathode material and corresponding electronic band strcuture as obtained by DFT.

Goal: The project will focus on the computational investigation of **new and unexplored compounds for cathode materials in sodium-ion batteries.** Apart from the investigation of known structures and compositions, the project aims on proposing suited candidate materials for detailed experimental investigation. The computational study will focus on the usage of quantum mechanical ab initio methods (density functional theory) to investigate structural stability (specific capacity, voltage profile), electronic properties (band structure) and diffusion behavior (diffusion barriers). The project will be in close cooperation with Dr. Anji Reddy Munnangi (HIU), who will do synthesis and characterization of computationally promising materials.

Note: Interest in quantum mechanics and computer simulation are prerequisites. Simulations will be conducted in a linux environment (knowledge in or willingness to learn linux are therefore necessary). The work will be under the guidance of Dr. Holger Euchner (HIU) and supervised by Prof. Axel Groß (Institute of Theoretical Chemistry, Ulm University).

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