Computational Workflows for an Accelerated Design of Novel Materials and Interfaces

Ivano E. Castelli

Department of Energy Conversion and Storage, Technical University of Denmark, Anker Engelundsvej 411, DK-2800 Kgs. Lyngby, Denmark

ivca@dtu.dk

The development of automated computational tools is required to accelerate the discovery of new functional materials, to speed up the transition to a sustainable future. Here, I address this topic by designing new electrodes with controlled interfaces for different applications which accelerate the transition to a sustainable future. These workflows are implemented in the framework of Density Functional Theory, using MyQueue and the Atomistic Simulation Environment (ASE). In the first part, I describe a fully autonomous workflow, which identifies materials to be used as intercalation electrodes in batteries, based on thermodynamic and kinetic descriptors like adsorption energies and diffusion barriers [1]. A substantial acceleration for the calculations of the kinetic properties has been obtained due to a recent implementation of the Nudged Elastic Bands (NEB) method, which takes into consideration the symmetries of the system to reduce the number of images to calculate. Moreover, we have established a surrogate model to identify the transition states, which can further reduce the computational cost to at least one order of magnitude [2, 3]. We have applied this workflow to discover new cathode materials for Mg batteries as well as solid state electrolytes for Li, Na, and Mg all-solid-state batteries [1, 3]. In the second part of my talk, I discuss how engineering the interface can positively impact surface properties. I show this concept using two examples. In the first one, I nanostructure materials to increase the Li-storage capacity in C-anodes or to adjust the change in volume during charge/discharge in Si-anodes for Li-ion batteries [4]. In the second example, I apply strain engineering and external stimuli to switch material's polarization to decrease the reaction overpotential in oxynitride materials for the oxygen evolution reaction [5, 6].

References

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