PREDICTION OF STABILITY AND VOLTAGE OF LAYERED OXIDE MATERIALS FOR SODIUM-ION BATTERIES

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Keywords: Classical Potential • DFT • Continuum • Cathode • Sodium-Ion Batteries

Abstract: Layered oxides (LOs) are among the most promising cathode materials for Na-ion batteries (SIBs) because of their potentially high energy densities. There are, however, still some challenges in applying LO cathodes for SIBs, in particular because of their low cyclability, which is mainly related to their structural evolution (i.e. phase transition). We have recently developed an efficient Coulomb energy optimizer using advanced sampling methods. Our optimization package, GOAC (Global Optimization of Atomistic Configurations by Coulomb), can achieve a speed up of several orders of magnitude compared to existing softwares and more importantly can be used to sample gigantic configurational spaces of up to ten to the power of several thousands configurations. By applying our software package GOAC we optimized Coulomb energies in complex multi-element LOs ($Na_x[M_yM'_{1-y-\dots}\dots]O_2$) to simulate their phase stability and transition during charge/discharge. The predictive capability of this approach will be discussed. Besides the cationic potential, which has been reported before by other groups, we found other parameters that determine the phase stability of LOs. Afterwards, our recently developed classical potential to predict the voltage profile *V(x)* of LOs will be presented. It is shown that *V(x)* can be computed with a high accuracy. Parameters controlling the voltage range and plateaus, which influence the stability of LOs, will be discussed. Finally, our multiscale modelling and simulation studying the mechanism of cracking in LOs by desodiation/sodiation will be presented. In particular, the influence of composition on the mechanical stability will be discussed.