A density functional theory study of the carbon-coating effects on lithium iron borate battery electrodes

Lithium iron borate (LiFeBO₃) is a promising cathode material due to its high theoretical specific capacity, inexpensive components and a small volume change during operation. Yet, challenges relating to severe air- and moisture-induced degradation necessitate the application of a protective coating on the electrode which also improves the electronic conductivity. However, not much is known about the preferential geometries of the coating as well as how these coating-electrode interfaces influence the lithium diffusion between the coating and the electrode. Here, we therefore present a density functional theory (DFT) study of the anchoring configurations of carbon coating on the LiFeBO₃ electrode and its implications on the interfacial lithium diffusion. Due to large barriers associated with Li-ion diffusion through a parallel-oriented pristine graphene coating on the FeBO₃ and LiFeBO₃ electrode surfaces, large structural defects in the graphene coating are required for fast Li-ion diffusion. However, such defects are expected to exist only in small concentrations due to their high formation energies. Alternative coating geometries were therefore investigated, and the configuration in which the graphene coating layers were anchored normal to the electrode surface at B and O atoms were found to be most stable. Nudged elastic band (NEB) calculations of the lithium diffusion barriers across the interface between the optimally oriented coating layers and the electrode show no kinetic limitations for lithium extraction and insertion. Additionally, this graphite-coating configuration showed partial blocking of electrode-degrading species.