Multiscale phase field modeling for the description of conversion reactions in lithium ion and lithium air batteries

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The development of theoretical methods to correlate the chemical and structural properties of electrode materials with their electrochemical behavior in energy storage devices is of crucial importance for consistent interpretation of experimental data and for their optimization toward end-user applications [1,2].

This lecture discusses available techniques to integrate *ab initio*-extracted parameters into phase field models describing solid phase formation and separation in materials and reactions relevant for lithium ion and lithium air batteries. In particular, a new model is presented which extends a previous approach extensively developed for the multiscale modeling of fuel cells [2-4]. The model is designed to take into account the on-the-fly multiscale coupling between continuum models describing ionic transport across the batteries electrodes andAllen-Cahn and Cahn-Hilliard –based phase field electrochemical models parametrized with DFT data [5-6] describing solid phase formation and separation (e.g. CoO/Co°/Li_2O in lithium ion batteries, and Li_2O/Li_2O_2/LiO_2 in lithium air batteries) during charge and discharge.Results are presented, and concepts, methods and challenges of this type of approaches are discussed.

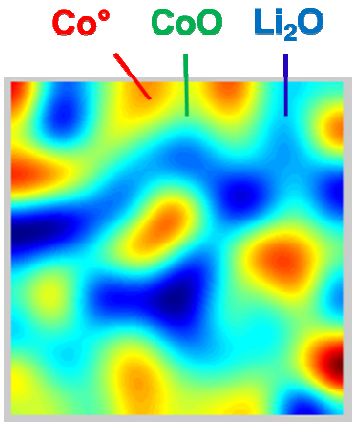

Figure 1: Example of phase field simulation result for the Co°/CoO/Li_2O system.

References

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