MAR17-2016-020021

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

Defect physics as key to understanding complex battery electrode materials

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In complex functional materials such as those for metal-ion battery electrodes, point defects can be vital or fatal to the performance. A detailed understanding of the formation and migration of these defects is thus required for explaining, predicting, and optimizing the materials' properties, and for rational materials design. With advances in electronic-structure methods, first-principles calculations for defects have become a powerful tool in providing such an understanding. In this talk, I will focus my discussion on defect physics vis-à-vis functional properties in mixed ionic-electronic conducting, electrode materials. Specific examples will be taken from recent work on complex transition-metal oxides. Through these examples, I will illustrate how state-of-the-art point defect calculations can serve as a study of materials response to interventions, done on purpose and in a well-controlled manner, at the electronic and atomic level, and how such a study can provide a fundamental understanding of the materials and help uncover new science.