An Atomistic and Mesoscale Perspective of Multivalent Intercalation Batteries: Challenges in Cathode and Anode Design

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The deficiencies of electrochemical energy storage are a major constraint in many areas of technological design. Using a canonical intercalation host, V_2O_5, as a model system, I will first discuss the structural and electronic origins of diffusion barriers in cathode materials. Scanning transmission X-ray microscopy measurements in conjunction with resonant inelastic X-ray scattering and density functional theory provide a rich picture of the evolution of electronic structure with increasing intercalation. The mitigation of diffusion impediments will be discussed with reference to the stabilization of metastable phases that provide frustrated coordination environments and enable the relatively facile diffusion of polarons. This approach has led to the discovery of several promising intercalation hosts for Mg- and Ca-ion batteries. I will focus on a tunnel-structured ζ-V_2O_5 polymorph that provides an unprecedented combination of high voltage, excellent cyclability, and good capacity and will discuss further elaboration of this concept to other polymorphs of V_2O_5.

A promising advantage of switching to Mg-based batteries derives from the many reports which claim that Mg is inherently non-dendrite forming. I will address the issue of whether Mg is truly impervious to dendritic growth. The targeted navigation of electrodeposition landscapes to achieve controllable film morphologies will also be discussed, and holds potential for yielding low-volume expansion, lower current density anode materials.