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Connecting the dynamic response of electrodes to their electronic structure

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The electrodes of Li-ion batteries exhibit a wide range of intriguing electronic, thermodynamic and kinetic properties. Most electrode materials undergo a series of phase transformations as a result of drastic changes in Li concentration during each charge and discharge cycle. The mechanisms of these phase transformations remain poorly understood but usually involve a coupling between ionic diffusion, structural changes and interface migration. While phase transformations affect electrodes at the particle level, their mechanisms are ultimately determined by the electronic structure and crystallography of the electrode chemistry. Describing these phase transformations phenomenologically starting from first principles requires suitable coarse-graining strategies and a reliance on statistical mechanical approaches to account for the important role of temperature and entropy. This talk will describe how first-principles statistical mechanical approaches have provided insights about the mechanisms of kinetic processes in a variety of transition metal oxides and sulfides with widely differing crystal structures.