1116-74-744 **Michael L. Falk*** (mfalk@jhu.edu), **Tonghu Jiang**, **Shiva Rudraraju** and **Krishna Garikipati**. *The materials science of chemically driven elastic incompatibility: A multi-physics study of lithium ion battery electrode Li1+xT2O4.*

Recently, a huge materials space is being explored for cheaper, higher energy density, and reliable battery materials, due to the growing demand of portable electronics and electric vehicles. During charge and discharge cathodes of lithium ion batteries typically undergo first order phase transformations. The resulting two-pahse coexistence can lead to elastic incompatibilities that drive failure and limit lifetime.

In this work, we use a series of computational tools to study the thermodynamics and kinetics of Li1+xTi2O4. Density functional theory (DFT) calculation was used to obtain formation energies of Li1+xTi2O4 with different lithium configurations, and migration barriers for lithium ion transitions. The cluster expansion method is employed to approximate these energies. These are then deployed to develop physics-based parameterizations of the relevant structural and kinetic properties that inform a phase field model in order to simulate this material at macroscopic level. The development of internal stresses during charging and discharging is simulated and analyzed with an eye to understanding how these lead to electrode degradation and failure. (Received September 11, 2015)