Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

A multi-physics study of Li-ion battery material $\mathbf{Li_{1+x}Ti_2O_4}$
TONGHU JIANG, MICHAEL FALK, Johns Hopkins University, KRISHNA SIVA SHANKAR RUDRARAJU, KRISHNA GARIKIPATI, ANTON VAN DER VEN, University of Michigan — Recently, lithium ion batteries have been subject to intense scientific study due to growing demand arising from their utilization in portable electronics, electric vehicles and other applications. Most cathode materials in lithium ion batteries involve a two-phase process during charging and discharging, and the rate of these processes is typically limited by the slow interface mobility. We have undertaken modeling regarding how lithium diffusion in the interface region affects the motion of the phase boundary. We have developed a multi-physics computational method suitable for predicting time evolution of the driven interface. In this method, we calculate formation energies and migration energy barriers by ab initio methods, which are then approximated by cluster expansions. Monte Carlo calculation is further employed to obtain thermodynamic and kinetic information, e.g., anisotropic interfacial energies, and mobilities, which are used to parameterize continuum modeling of the charging and discharging processes. We test this methodology on spinel $Li_{1+x}Ti_2O_4$. Elastic effects are incorporated into the calculations to determine the effect of variations in modulus and strain on stress concentrations and failure modes within the material. We acknowledge support by the National Science Foundation Cyber Discovery and Innovation Program under Award No. 1027765.

Tonghu Jiang
Johns Hopkins University

Date submitted: 19 Dec 2012 Electronic form version 1.4