Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Car-Parrinello molecular dynamics study of the charge-discharge cycle in lithium-ion battery materials Y. F. KUNG, C.J. JIA, SIMES, SLAC National Accelerator Laboratory and Stanford University, W. E. GENT, Stanford University, I. LEE, SIMES, SLAC National Accelerator Laboratory and Stanford University, B. MORITZ, SIMES, SLAC National Accelerator Laboratory, T. P. DEVEREAUX, SIMES, SLAC National Accelerator Laboratory and Stanford University — Lithium-ion transition metal oxide compounds have shown great potential for use as battery electrodes. However, the underlying structural modifications which accompany delithiation during battery charging remain less well understood. Formation of peroxide-like species and cation migration between layers comprise two promising candidates for describing numerous experimental observations. Taking Li_2RuO_3 as a model system, we use Car-Parrinello molecular dynamics to examine the structural changes that occur during delithiation and lithiation. We compare our results to existing experimental observations in other compounds and provide guidance for future experiments, including resonant inelastic x-ray scattering (RIXS).

Yvonne Kung
Stanford University

Date submitted: 11 Nov 2016 Electronic form version 1.4