Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

First Principles Investigation of Li/Fe-Oxide as a High Energy Material for Hybrid All-in-One Li-ion/Li-O_2 Batteries ALPER KINACI, LYNN TRAHEY, MICHAEL M. THACKERAY, Argonne National Laboratory, SCOTT KIRKLIN, CHRISTOPHER WOLVERTON, Northwestern University, MARIA K.Y. CHAN, Argonne National Laboratory, CENTER FOR ELECTRICAL ENERGY STORAGE COLLABORATION — We recently introduced a vision for high energy all-in-one electrode/electrocatalyst materials that can be used in hybrid Li-ion/Li-O_2 (Li-air) cells [1]. Recent experiments using Li_5FeO_4 demonstrated substantially smaller voltage polarizations and hence higher energy efficiency compared to standard Li-O_2 cells forming Li_2O_2 [2]. The mechanism by which the charge process activates the Li_5FeO_4, however, is not well understood. Here, we present first principles density functional theory (DFT) calculations to establish the thermodynamic conditions for the extraction of Li/Li+O from Li_5FeO_4. A step-by-step, history-dependent, removal process has been followed and the stability of the Li and Li+O deficient samples is investigated on the basis of the energies of the extraction reactions. Various stages of Li/Li+O removal are identified, and structural changes and electronic structure evolution, as well as computed XRD, XANES, and PDF characterizations are reported.

[1] M. M. Thackeray, M. K. Y. Chan, L. Trahey, S. Kirklin, and C. Wolverton, Journal of Physical Chemistry Letters, 4, 3607 (2013).
[2] L. Trahey, C. S. Johnson, J. T. Vaughey, S.-H. Kang, L. J. Hardwick, S. A. Freunberger, P. G. Bruce, M. M. Thackeray, Electrochemical and Solid-State Letters, 14, A64 (2011).

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Date submitted: 15 Nov 2013 Electronic form version 1.4