Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

First-principles study of $LaSn_3$ as an anode for lithium-ion batteries DONGWON SHIN, CHRISTOPHER WOLVERTON, Northwestern University, JOHN VAUGHEY, MICHAEL THACKERAY, Argonne National Laboratory —
Using both density functional theory (DFT) calculations and experiment, we investigate the tin-rich intermetallic compound $LaSn_3$as a possible anode for lithium-ion batteries. We use DFT calculations to compare the relative energies of hypothetical insertion- and displacement-type reactions in an effort to elucidate the energetically-preferred reaction mechanism of Li with $LaSn_3$. From our DFT calculations, we find: (i) lithium insertion reactions with $LaSn_3$ are predicted to be energetically unfavorable and highly unlikely to occur; (ii) in contrast, the energetically preferred reaction is a displacement reaction in which La is partially displaced from $LaSn_3$ to yield La_3Sn_5 and Li reacts with the residual Sn to form $Li_{17}Sn_4$, corresponding to an electrochemical capacity of 307 mAh/g (iii) this partial displacement reaction is preferred relative to the complete displacement and lithiation of Sn; and (iv) the lithiated-tin compound, $Li_{17}Sn_4$, is energetically more favored than the commonly reported $Li_{22}Sn_5$ composition. Electrochemical and structural data largely confirm the DFT predictions; they demonstrate that lithium reacts with $LaSn_3$ via a displacement reaction to provide a reversible specific capacity of 200-250 mAh/g.

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Date submitted: 22 Nov 2008 Electronic form version 1.4