First-principles study of LaSn₃ as an anode for lithium-ion batteries  
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Using both density functional theory (DFT) calculations and experiment, we investigate the tin-rich intermetallic compound LaSn₃ 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 LaSn₃. From our DFT calculations, we find: (i) lithium insertion reactions with LaSn₃ 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 LaSn₃ to yield La₃Sn₅ and Li reacts with the residual Sn to form Li₁₇Sn₄, 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, Li₁₇Sn₄, is energetically more favored than the commonly reported Li₂₂Sn₅ composition. Electrochemical and structural data largely confirm the DFT predictions; they demonstrate that lithium reacts with LaSn₃ via a displacement reaction to provide a reversible specific capacity of 200-250 mAh/g.

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