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Structural and Electrochemical Characterization of Silicon Clathrate Materials Upon Lithium Insertion

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Due to its high theoretical specific capacity, silicon has been the subject of intense interest and research as a high energy density anode for lithium-ion batteries. In the last several years, nanostructured silicon has been shown to be very effective for relieving lithiation induced strain and avoiding pulverization, which can lead to capacities > 3000 mAh/g, a 10X improvement over the commercially used graphite anode. However, despite this impressive proof-of-principle, nanostructured silicon can still suffer from degradation over long cycling times due to several reasons such as collapse of the nanostructure, increased porosity, structural instability, and insufficient surface passivation. The work to be presented here will introduce our investigations into the lithiation of silicon clathrates, (fullerene-like materials where silicon atoms are arranged in cage-like structures) that have been shown, through first principles calculations, to be able to allow lithium insertion without a large volume change or pulverization. The preliminary experimental results of lithiation into several silicon clathrate alloy materials will be presented and compared to lithiation of diamond cubic and amorphous silicon. The results of structural characterization using ex-situ X-ray diffraction, neutron diffraction, and X-ray photoelectron spectroscopy to understand the structural changes occurring in the clathrates during and after lithiation will also be discussed.