Title : Impact of Lithiation on Si-anode/binder interfaces for next generation Lithium ion batteries

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Abstract:

To achieve increased energy densities in lithium-ion batteries (LiBs), the intercalation chemistry must be replaced by anode materials that are capable of electrochemically alloying with lithium.
Silicon is one of the best candidate material for it, however it suffers from poor intrinsic conductivity and volumetric expansion [1, 2]. The use of polymeric binders [3, 4] have been proposed to maintain the structural integrity of the anode under cycling. Several research efforts have aimed at enhancing the mechanical, elastic, electrical, and ionic properties of binders for use in Si anodes [1, 3, 5, 6]. Silicon/polymer interfaces [7] are crucial for the anode performance. In this work we focus on some recently proposed polymers, functionalized with boronic acid groups (B-OH_PANI and a PVA crosslinked co-polymers.

We study, using a first-principles approach based on the Density Functional Theory (DFT), the mechanisms that determine the adhesion properties of the polymers to a Si (111) surface. The structural and electronic properties as well as the energetics of boronic acid doped polyaniline (B-OH_PANI) and polyvinyl alcohol (PVA) monomers [8] absorbed on the Si (111) surfaces before and after lithiation, have been investigated. We showed that the co-absorption of these two monomers increases the absorption energy and in general improves the adhesion properties of both polymers to the Si (111) facet. The structural evolution and corresponding electronic properties as a function of Li concentration will be discussed.

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