

## Analysis of Graphene Coating Effects on Si Anode during the Lithiation

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Computational study on the effect of graphene coating to Si anode material is performed by using density functional theory calculations. We construct the atomic model to examine interactions between amorphous silicon and graphene during lithiation. The lithiation of Si anode increases the mechanical contact force between outer graphene layer and amorphous silicon and the shear resistance is also increased. To explain the interaction between graphene and silicon we examine the charge distribution of silicon and graphene considering lithiation insertion. The number of density, electro field distribution and electric potential are also calculated. Charge-non polar interaction between Li-ion and graphene increase the contact energy between graphene-silicon. In addition, we investigate Graphene-coated silicon monoxide anode material which has similar electro-chemical characteristic but has positive charge state of oxygen. The same tendency is observed in silicon monoxide anode material. To calculate the contact force, we simplified interaction atomic force model. In this theoretical study, potential improvement of cyclability and improved mechanical properties of graphene coating for Si anode have been investigated.

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