

Sili-graphene a high capacity Anode material for Lithium-Ion Battery

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Abstract

In this study, we have proposed a anode material based on Silicon doped graphene (Siligraphene) for developing the Li-ion batteries (LIBs). We have predicted that Siligraphene can be an anode material for lithium batteries. In particular, we have found that the Siligraphene sheet can adsorb lithium atoms in different sites in hexagonal structure. Also, we have found that Lithium atoms can be diffused along the plane of siligraphene. The energy of diffusion of siligraphene (SiC₃) is about 0.095eV, for Li on top of silicon atoms is about 0.223eV, indicating rapid charging/discharging processes. During charging and discharging the electrode Li_xSiC₃ exhibit small variation in voltage and makes them a potential candidate for Li-ion batteries.

Biography:

Dr.M. Houmad was interested in DFT calculationsOptical properties2D MaterialsMaterials for energynano-materials.

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