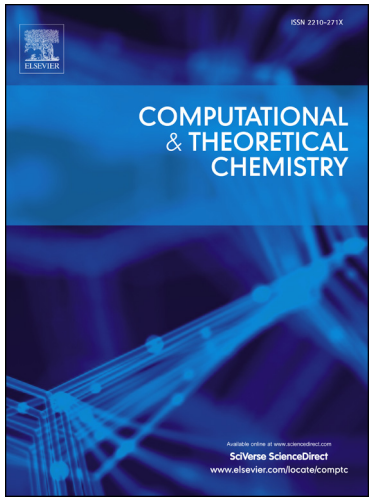

First-Principles Study of Lithium Insertion into $Si_{10}H_{16}$ Cluster

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First-Principles Study of Lithium Insertion into $Si_{10}H_{16}$ Cluster

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Abstract Due to the high theoretical capacity of silicon for lithium storage, it has been intensively studied as an anode material for lithium-ion battery. However the large volume expansion due to insertion of lithium hampers its practical application. The understanding of reaction mechanism is crucially important to solve the large volume change problem of silicon. We built up a hydrogen-passivated silicon atomic cluster ($Si_{10}H_{16}$) as a model and then theoretically studied the influence of lithium adsorption on its electronic and crystal structures based on the density functional theory. Investigation of the structure and physical properties of silicon atomic cluster upon lithium adsorption can help to explain the phenomena such as insertion mechanism and surface diffusion process, since most of the atoms in the atomic cluster could be looked as sitting at the surface. The results showed that the insertion of lithium will weaken the Si-H bond and push the closest Si atom away. The diffusion process of lithium into $Si_{10}H_{16}$ along the tetrahedral sites have also been investigated, the data indicated that the diffusion barrier has close relationship with the coordination number around the inserted lithium.

Keywords: Si atomic cluster; Li insertion; Electronic structure; Diffusion process.

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