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# First-principles calculations on lithium and sodium adsorption on graphene edges

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**Abstract**

Porous hard carbons are known for their high specific capacities in lithium (Li) and sodium (Na) storage. Due to lack of layered graphitic structure but abundance of pores and high specific surface areas, the hard carbons are believed to mainly adsorb the Li and Na atoms on the surfaces of their pores rather than store them between the graphene layers. Various models have been proposed and the density functional theory (DFT) calculations have been carried out, but the mechanism of Li and Na storage in these materials is still unclear due to the complicated structure of the hard carbons. In this article, the Li and Na storage is simulated by considering various configurations of Li and Na atom adsorption on pure graphene edges. It shows that, with increasing number of the adsorbed atoms, the Li and Na atoms are firstly strongly adsorbed on the edges and then adsorbed near the edges. Finally, they become condensed on the edges and form a quasi-metal or metal. These findings help to understand the mechanisms of Li and Na adsorption in the hard carbons, to guide the structural design of porous hard carbons and to improve their Li and Na storage performances.

**Keywords:** adsorption, porous hard carbons, graphene, density functional theory