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### Aluminum functionalized few-layer silicene as anode material for alkali metal ion batteries

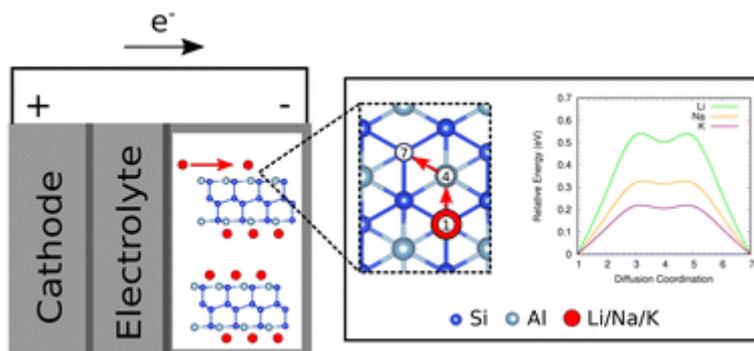


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#### Abstract

We have investigated the possibility of using aluminum functionalized silicene trilayers (ABC-Si<sub>4</sub>Al<sub>2</sub>) as an anode material for alkali metal ion batteries (AMIBs). First, we studied the thermodynamic stability of ABC-Si<sub>4</sub>Al<sub>2</sub> using *ab initio* molecular dynamics simulations, showing that this material remains stable up to around 600 K. Then, we explored the properties of alkali metal atoms (Li, Na, K) adsorption in ABC-Si<sub>4</sub>Al<sub>2</sub>, finding several available sites with high average adsorption energies. Moreover, we computed the diffusion properties of those adsorbed atoms along high-symmetry paths using the nudged elastic band method. The results indicated diffusion barriers as low as the ones in graphite, especially for Na (0.32 eV) and K (0.22 eV), which allows those ions to migrate easily on the material's surface. Our studies also revealed that the full loaded Li<sub>4</sub>Si<sub>4</sub>Al<sub>2</sub>, Na<sub>2</sub>Si<sub>4</sub>Al<sub>2</sub>, and K<sub>2</sub>Si<sub>4</sub>Al<sub>2</sub> systems provide low average open-circuit voltage, ranging from 0.14 to 0.49 V, and large theoretical capacity of 645 mAh g<sup>-1</sup> for Li- and 322 mAh g<sup>-1</sup> for Na- and K-ion batteries, values that are close to the ones in other anode materials, such as graphite, TiO<sub>2</sub>, and silicene-based systems. Those results indicate that aluminum functionalized few-layer silicene is a promising material for AMIBs anodes, particularly for Na- and K-ion batteries.

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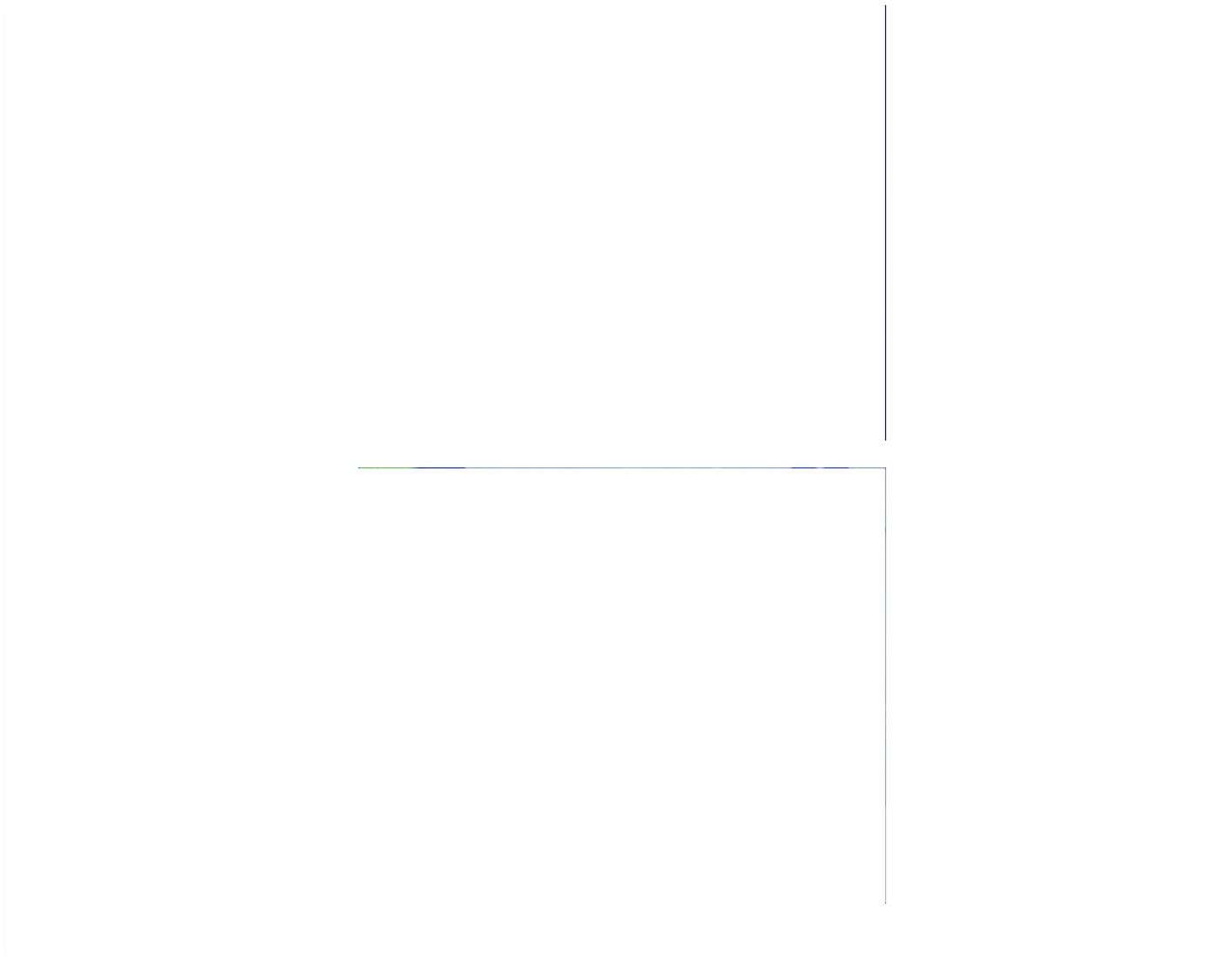
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