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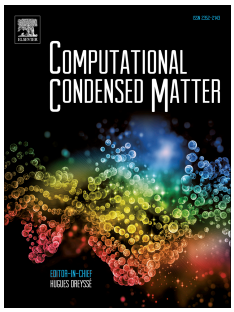

Mono and bi-layer germanene as prospective anode material for Li-ion batteries: A first-principles study

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Mono and bi-layer germanene as prospective anode material for Li-ion batteries: A first-principles study

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Abstract

To find suitability of two dimensional (2D) mono-layer (ML) and bi-layer (BL) germanene as anode material for Li-ion batteries (LIBs), a series of first-principles calculations based on density functional theory (DFT) have been carried out. Our calculations suggest that adsorption of Li atom at hollow site of germanene is energetically favorable. The role of strain on formation energy has been extensively studied for fully lithiated ML and BL germanene. The Bader charge analysis indicates that the transfer of charge occurs from adsorbed Li atom to 2D germanene sheet, suggesting the formation of ionic bond between Li and Ge atom. We have calculated capacity during discharge cycle of fully lithiated ML and BL germanene sheet equals to **369** mAhg^{-1} and **276** mAhg^{-1}, respectively. The average intercalation voltage (AIV) of Li-ion has been calculated for ML and BL germanene. We utilized the climbing image nudged elastic band (CI-NEB) method to analyze the energy barrier for Li-ion diffusion along the surface and through the germanene sheet. In order to find stability of Li adsorbed germanene at high temperature, we have performed $ab-initio$ molecular-dynamics (AIMD) calculations at 300 K.

Keywords: A. DFT; B. Nano material; C. Electrochemical properties; D. Li-ion batteries

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