Abstract Submitted
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Computational design and point defects engineering in two-dimensional silicene and germanene.[1] YULIANG MAO, Xiangtan Univ — We present first-principles results of a new type hybrid phases composed by buckled germanene with saturated or half-saturated alkali metal atoms adsorption. Our energetics and electronic structure analysis suggests that adsorbed alkali metal atoms (Li, Na, K) can be used as covered adatoms to synthesize germanene-based new phases in two dimensional. Charge transfer is significant between the alkali metal atoms and Ge, indicating the ionic interactions between them. Furthermore, our charge density analysis indicates that covalent component in some extent exists in Ge_2X_2 and Ge_2X_1 (X = Li, Na, K) 2D phases, which even leads the complete lithiated germanene into a semiconductor with an energy gap of 0.14 eV. We report that 2D phases of Ge_2X_1 (X = Li, Na, K) are metallic with weak polarization on the Fermi level and in unoccupied states. We also performed spin-polarized calculations to design the lithium storage material by using the active edges of zigzag silicene nanoribbon. We predict that edge-adsorpion of Li adatoms on zigzag silicene nanoribbon is preferred in energy to form new type lithium storage materials.

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