

# Graphene-analogous Siligene (2D SiGe) as Anode Material for Alkali Metal Ion Batteries

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The group IV elements, especially silicon (Si) and germanium (Ge), are promising candidates for anode materials for the next-generation lithium, sodium, and potassium batteries, because of their high theoretical capacity. However, their commercialization is greatly hindered due to a large volume expansion on lithiation, a low Coulombic efficiency of Si anode, and low abundance and high cost of Ge. Therefore, it is believed that the incorporation of Ge in Si can improve the electrochemical performance of battery significantly.[1, 2] Experiments show that nanostructure SiGe-based anodes have high rate capabilities, improved cycle lives and enhanced capacity retentions in LIBs.[2-4] Herein, using the density functional theory, we propose that the SiGe monolayer (siligene) can be a universal anode material for alkali metal (Li, Na, and K) ion batteries. The phonon dispersion and cohesive energy manifest the dynamic and thermal stability of a SiGe monolayer. All the metal atoms considered preferably adsorb above the center of the holes of honeycomb lattice with a strong binding energy. The SiGe monolayer provides moderate/low migration energy barriers for the alkali metal atoms (0.14 - 0.36 eV), suggesting fast charge/discharge rates and longer cycle life. We show that the pristine SiGe possesses the Dirac cone-shaped linear band dispersion with a small gap of 12 meV at the 'K' point.[5] The adsorption of a single alkali metal atom changes this semiconducting nature to metallic state due to a significant charge transfer from the outermost s-orbital of alkali metal atoms to the substrate. This trend remains intact at a low coverage of Li, but upon full lithiation (on both side of SiGe,  $\text{Li}_2\text{SiGe}$ ), a two-step charge transfer process occurs which reopens the band gap, as the initial pristine siligene. We find that the system is metallic up to Li coverage of 1.5 ( $\text{Li}_{1.5}\text{SiGe}$ ), yielding a storage capacity of  $383 \text{ mAh g}^{-1}$ . However, even at a high coverage, Na and K do not follow this trend. Thus, the calculated theoretical capacities for Na and K ions are 1064 and  $532 \text{ mAh g}^{-1}$ , respectively, which are larger than that of other 2D anode materials. The calculated low average voltages ensure the suitability of SiGe monolayer as a prospective anode for alkali metal ion batteries.

## References:

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