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Density Functional Theory Studies of Li-ion interaction with defected group 14 heteronuclear nanotubes and nanosheets TICHAKUNDA PASIPANODYA, PRABATH WANAGURU, RAYMOND ATTA-FYNN, University of Texas at Arlington — Nanomaterials show significant promise in enhancing Lithium ion (Li-ion) battery properties. Using density functional theory, we study the binding and diffusion of Li on defected nanotubes and nanosheets of silicon carbide (SiC) and silicon germanium (SiGe). Point and extended defects are considered to fully evaluate the influence of defects on the adsorption and diffusion properties. The trends in the adsorption-induced changes in the geometric and electronic properties will be presented. Furthermore, room temperature ab initio molecular dynamics simulations will be carried out to investigate finite temperature effects on the binding mechanisms and electronic structure.

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