

Abstract Submitted
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Interaction of a single Li atom with SiGe(6,6) nanotubes¹ PRABATH WANAGURU, ASOK K. RAY, University of Texas at Arlington — A study of the interaction between four types of SiGe(6,6) nanotubes² and a Li atom was performed using the cluster approximation. Full geometry and spin optimizations were performed without any symmetry constraints using the hybrid functional B3LYP, an all electron 6-311G**//3-21G* basis set and the GAUSSIAN 09 suite of software. All possible internal and external adsorption sites were considered and it was found that some tubes were deformed as a result of the adsorption process. Among the nanotubes which retained the tubular shape, most preferred site for the external adsorption was quasi on top of Ge site with the highest adsorption energy being 1.639eV. Also, the band gaps of the systems decreased from the values of pristine SiGe nanotube values, the range being 0.880 to 0.958eV. For inside adsorption, most preferred site was the hollow site. Adsorption energies ranged from 1.606 to 1.657eV and band gaps, from 0.777 to 0.807eV. We will present, In detail, adsorption energies, band gaps, density of states, and the bonding nature of Li to the nanotubes.

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Prabath Wanaguru
University of Texas at Arlington

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