

Abstract Submitted
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Interaction of Si atoms and Si-based radicals with carbon nanotubes and graphene monolayers¹ KISEOK CHANG, SAVAS BERBER, DAVID TOMÁNEK, Michigan State University — We use *ab initio* density functional calculations to study the interaction of Si atoms and Si-based radicals, such as SiH₃, with single-wall carbon nanotubes and graphene monolayers. We find that both Si atoms and radicals form a strong chemisorption bond, accompanied by a small relaxation and a locally increased sp³ bond character of the graphitic nanostructure. We identify the optimum adsorption geometries at different adsorbate coverages and adsorbate-related changes in the electronic structure and vibration spectra of the systems. We propose that successful functionalization of carbon nanotubes or graphene by Si atoms or Si-based radicals can be verified by studying changes in the radial breathing mode of nanotubes and the G-band of graphitic nanocarbons using Raman spectroscopy.

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Kiseok Chang
Michigan State University

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