Abstract Submitted
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Ab initio **study of semiconducting carbon nanotubes adsorbed on the Si(100) surface: diameter- and registration-dependent atomic configurations and electronic properties**[1] SALVADOR BARRAZA-LOPEZ, PETER M. ALBRECHT, NICHOLS A. ROMERO[2], KARL HESS, University of Illinois — We present a theoretical study within density functional theory in the local density approximation of semiconducting carbon nanotubes adsorbed on the unpassivated Si(100) surface. We find that the interaction between the nanotube and silicon surface results in significant atomic re-arrangment of the surface atoms. Since the spatial configuration of the surface dimers determines to a great extent the electronic properties of the surface, our first-principles calculations indicate a tendency towards metallicity for the semiconducting tube-Si(100) surface system. We confirm this for nanotubes of different diameters and chiral angles, and find the effect to be independent of the orientation of the nanotubes on the surface. Reference: cond-mat/0510477 and references therein.

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