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Electronic structure of carbon nanotubes adsorbed on Si(001) vicinal surfaces. S. BERBER, A. OSHIYAMA, University of Tsukuba — We have investigated adsorption of carbon nanotubes on Si(001) vicinal surfaces using Density Functional Theory total energy and electronic structure calculations. Energetically favorable adsorption orientations and positions of carbon nanotubes were searched by total energy calculations, and detailed atomic structure of carbon nanotubes adsorbed at most probable adsorption sites have been obtained by full structure relaxation. Adsorption energy shows both direction and site dependence since the carbon nanotube form covalent bonds with the clean vicinal surface. Charge transfer between the nanotube and the surface happens mainly at the interface, which results in a quasi one-dimensional electron channel. Electronic states of carbon nanotube and silicon surface are highly rehybridized and mixed. A metallic carbon nanotube could behave as small gap semiconductor depending on adsorption site. Insertion of sp^3 bonded carbon atoms in sp^2 bond network introduces energy gap in electronic structure of the nanotube near Fermi level. This energy gap could be eliminated if there are surface states available for charge transfer. But such surface states are not available for particular nanotube directions, and non-metallic electronic structure appears. Dangling bond states of silicon surface, which appears as energy bands near the Fermi level, attracts electrons from the nanotube provided that these states are localized near the nanotube. Termination of surface dangling bonds in the vicinity of adsorbed nanotube could help tune the electronic properties of adsorbed nanotube.

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