

Abstract Submitted
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Stability of finite single-walled carbon nanotubes adsorbed on Si(001)¹ WALTER ORELLANA, Facultad de Ciencias Fisicas, Universidad Andres Bello — The stability and bonding properties of capped single-walled carbon nanotubes (CNTs) adsorbed on the Si(001) surface are studied using ab initio methods. Supercell calculations of finite CNTs on surface avoid the commensurability condition that an infinite CNT-surface system requires, providing a realistic description of bond formations. We consider capped armchair (5,5) and zigzag (9,0) CNTs with lengths of about 24 Å, adsorbed parallel and perpendicular to the Si-dimer direction of Si(001). At the equilibrium geometry we observe the formation of C-Si covalent bonds throughout the CNT-surface interface with binding energies ranging from 0.4 to 0.6 eV per C-Si bond. These bonds only form when nearest-neighbor C and Si atoms are closer than 2.15 Å. Our results show a preferential direction for the CNT adsorption along the Si dimers, where the zigzag CNT is found to be the most stable. We also find that the stability of the adsorbed CNTs depends to a major extent on the C-Si bond length instead of the numbers of bonds throughout the nanotube-surface interface.

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Walter Orellana
Facultad de Ciencias Fisicas, Universidad Andres Bello

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