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Diameter-Selective Alignment of Carbon Nanotubes on Si (001) Stepped Surfaces BATNYAM ENKHTAIVAN, MASAHIDE YOSHIMURA[1], JUN-ICHI IWATA, ATSUSHI OSHIYAMA, Department of Applied Physics, The University of Tokyo — The necessity of aligning carbon nanotube (CNT) raises important questions of whether the alignment is energetically feasible and of whether the electronic properties of CNTs are modified on the substrate surface. We report total-energy electronic-structure calculations based on the DFT that provide stable adsorption sites, structural characteristics, and energy bands of CNTs adsorbed on the Si(001) stepped surfaces. We choose (5,5), (9,9) and (13,13) armchair CNTs with the diameters of 6.8 Å, 12.2 Å and 17.6 Å and explore all the possible adsorption sites either on the terrace or at step edges. We find that the (9,9) CNT is most favorably adsorbed at the edge of the double-layer step D_B along the <110> direction, whereas the (5,5) and (13,13) CNTs favor the terrace site where the CNTs are perpendicular to the Si dimer rows. This finding is indicative of the diameter-selective self-organized alignment of CNTs by exploiting the Si surface steps. We also find that the electronic structure of each CNT is modified upon adsorption depending on the adsorption site and the diameter of the CNTs. In particular, the (9,9) CNT at the most stable step edge site becomes semiconducting and also an interesting flat band appears at Fermi level.

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