172g Effect of Metal Adsorption on the Band Structure of Semiconducting Nanotubes

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Semiconducting single wall carbon nanotubes (SWCNT) are being extensively investigated for their applications as channels for field effect transistors (FET's); issues remain unsolved regarding the metallic contact to the nanotube, such as the correct metal suitable to reduce the Schottky barrier and the effect of the metal adsorbates in the electrical characteristics of the nanotube. In this work we report ab initio studies of the adsorption of Cu, Au, and Pd atoms as well as benzene molecules in an infinite long (8,0) SWCNT. This is achieved by applying one-dimensional periodic boundary conditions to a unit cell containing the adsorbate and a piece of the SWCNT. The PW91 functional is used for the exchange and correlation with basis sets such as 6-31G* and LANL2DZ as implemented in the program Gaussian 03. Figure 1 shows 5 unit cells with gold adsorbates. The presence of the adsorbates reveals alterations in the optimized geometries whose effect on the band structure, thus electron velocities, are analyzed.