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Density Functional Theory Design of All-metallic Single-wall Carbon Nanotubes[1] LI CHEN, SWASTIK KAR, SAROJ NAYAK, Rensselaer Polytechnic Institute, PULICKEL AJAYAN, Rice University — We have used density functional theory to investigate the structure and electronic properties of Pt nanocluster decoration of single-wall carbon nanotubes (SWNTs). Energy optimization shows that Pt prefers to form clusters rather than spread out and "wet" the SWNTs. Atom-by atom increase in the cluster size is associated with the appearance of a number of new bands in the electronic structure, especially near the Fermi level. These new bands serve to modify the density of states near the Fermi level. While metallic SWNTs remain metallic, semiconducting SWNTs lose their band-gap rapidly with the inclusion of more than 3 atoms per cluster, and continue to remain metallic for all tested cluster sizes (n=0-13 and 19). Room temperature (T=300K) calculations of conductance show that SWNTs of different chiralities (both metallic and semiconducting) remain metallic for beyond n=3, with conductance close to $4e^2/h$. In some cases, the conductance is found to exceed this value. This gives an easy for designing "all-metallic" SWNT bundles.

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