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First-principles studies of electrical transport in metal-contacted semiconducting carbon nanotubes. JUAN PALACIOS, Universidad de Alicante (Spain), P TARAKESHWAR, DAE KIM, KIAS (South Korea) — We present first-principles calculations of the transport properties of semiconducting carbon nanotubes (CNT's), coupled to metallic electrodes. Our results indicate that, for realistic end-contact geometries, including atomic relaxation, the Fermi level position within the gap differs between palladium-contacted CNT's and gold-contacted CNT's. More interestingly, the contact resistance for the valence band in the case of Pd is much smaller than in the case of Au, while no significant difference is observed for the conduction band. This could explain experimental results showing that hole conduction is favored in the case of Pd contacts.

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