Extended Hückel theory for electronic transport in carbon nanotubes with metal contacts

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Extended Hückel theory (EHT) is a well established method for the description of the electronic structure of molecules and solids. Compared to density functional theory (DFT) it provides a good compromise between accuracy and computational burden.

In the present work we use a selfconsistent version of the EHT to study the electronic transport in metallic carbon nanotubes (CNTs) with various metallic electrodes (Al, Cu, Pd, Pt, Ag, Au). While the electronic structure of the metals is well described by the extended Hückel (EH) parameters of Cerdá [1], we show that a new parameter set for carbon strongly improves the agreement between EHT and DFT for small-diameter CNTs by taking into account the curvature of the tubes.

The new set of EH parameters for CNTs is developed by fitting the DFT band structure of the $(6,0)$ CNT [2]. Even though the new parameters are created for one unique CNT, they are highly transferable to all types of CNTs. To demonstrate the versatility of the approach, we compare selfconsistent EHT- and DFT-based electron transport calculations of finite length CNTs with metal electrodes. The good agreement between DFT and our new EHT is visible in the transmission spectra of the metal-CNT-metal systems. Furthermore, electronic transport properties of such systems are discussed in general. The conductance of metal-CNT-metal systems shows strong oscillations depending on the CNT length. This is attributed to finite-size effects. We find that the metals Ag and Au have the largest contact resistances to the CNT. Pd and Pt form low-Ohmic contact.

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