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Conductance of a Conjugated Molecule with Carbon Nanotube Contacts NICOLAS BRUQUE, University of California, Riverside, KHALID ASHRAF, THOMAS HELANDER, ROGER LAKE — Quantitative predictions of the energy levels is a well-known weakness of density functional theory (DFT). To understand the HOMO level alignment of a π-cruciform molecule [1] with the Fermi level of a carbon nanotube (CNT) contact, we have performed quantum chemical calculations of the adiabatic ionization potential (IP) of the central molecule. The adiabatic IP of the molecule is -5.86 eV. The image charge potential, calculated using our fully self-consistent DFT - Recursive Green Function (RGF) approach, is 0.7 eV. Treating the image potential as a self-energy correction to the IP, the HOMO energy level is at -5.16 eV which is comparable to the intrinsic CNT Fermi level at -5 eV. The above considerations of the energy level alignments, combined with the DFT-RGF analysis of the molecular orbitals and transmission spectrum, indicate that the HOMO resonance lies within the 50 meV energy window created by the experimental source-drain bias. This appears to be the most likely scenario that would give rise to the relatively small resistance of 6 MΩ.
1. X. Guo, et. al. Science, **311**, 356 (2006).

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