HUBBARD MODEL APPROACH TO THE ELECTRON TRANSPORT IN A MOLECULAR DEVICE

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9.7 cm

Electronic transport through a molecular device including benzene-like molecule connected to two semi-infinite leads is studied using the scattering approach. The molecule is described with the help of the single-orbital π-electron approximation with the electron interactions treated within the Hubbard model. The D-dimensional hypercubic leads (D=1, 2, 3) are described using the single band tight-binding model. The electron interactions in the molecule are treated by means of the Hartree-Fock approximation and the effects of selfconsistency on the transport properties of the device are analyzed in detail. The transmission function for a finite bias voltage is computed and the results are exploited to obtain I-V characteristics of the device. It is shown that the transmission is determined by the combined effect of the electronic structure of the molecule and the molecule-to-lead coupling. The Hubbard interaction neutralizes voltage-induced charge redistribution in the molecule which results in a shift of the transmission resonances and a substantial change of the current for intermediate values of voltage.

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