Electron Transport Through Atomic and Molecular Chains: Length Effects

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Abstract

Quantum transport and tunneling of electrons in an electrically biased, open quantum system is a nearly adiabatic, correlated, electron-molecule scattering process, with the Bloch wave boundary conditions of the metal leads applied to the scattering states. We generalize the tight-binding approach and, applying the methods of computational chemistry, we study the quasilinear transport of electrons through pi-conjugated organic polymer systems (oligo phenylen-viylene) as well as through monoatomic nanowires as function of the system length. We demonstrate that the proper placement of the electrostatic potential relative to the electrodes is important even for small bias voltages.

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