

Quantum interference effects on charge transport in molecular electronic junctions.

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The technological application of nanoscale functional elements made of individual molecules is a promising approach towards the miniaturization of electronic devices. In particular, there is a potential for exploiting quantum interference effects in controlling the charge transport in these molecular-scale devices.

The electronic conduction $G=I/V$ is determined by the electronic current I passing through a molecular junction from the left metallic lead to the right one and V is the voltage difference between the contacts. Current I is calculated based on the Landauer formula

$$I=(2e/h) \int_{(-\infty)^{\infty}} dE T(E) [f_{left}(E)-f_{right}(E)]$$

Here, $T(E)$ is the transmission coefficient, $f_{left}(E)$ ($f_{right}(E)$) is the Fermi distribution function of the left (right) metallic electrodes.

Our work is aimed at developing a theoretical approach that explains the effects of the conformation and intrinsic chemical nature of a molecule, the features of its electronic structure, and the geometry of its connection with metal electrodes on the efficiency of electronic conduction along this molecular wire.

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