INTERPLAY OF INTERFERENCE AND GEOMETRICAL EFFECT IN MOLECULAR BREAK JUNCTION

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We theoretically study the effects of functionalized molecular structures on the electronic transport of single-molecule junctions between Au electrodes [1]. The molecular structures are functionalized, in para and meta configuration, with methylsulfide anchor group on both or only one of their phenyl termini. We compared the results of transport calculations for molecular structures at zero and non-zero temperature. The molecular structures at zero temperature are obtained using the software *SIESTA* [2] for Density Functional Theory. Molecular structures at non-zero temperature are obtained using the software for molecular dynamics *lammps*. The Hamiltonians of the molecular structures of both zero and non-zero temperature are obtained using *SIESTA*. The transport calculations [3] are performed in the wide band limit [4]. Such approach is computationally efficient and allowed us to make a significant statistical study to account the effect of the temperature. We found that the thermal fluctuations enhance the effect of quantum destructive interference on the transport through the molecules functionalized in meta position.

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