

Abstract Submitted
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First-principles Time-dependent Density Functional Theoretical Approach for Quantum Transport of Molecular Electronic Devices

ZHONGYUAN ZHOU, SHIH-I CHU, Department of Chemistry, University of Kansas, Lawrence, KS 66045 — We present a first-principles time-dependent density functional theoretical approach that is computationally feasible for quantitative treatment of quantum transport of molecular devices. In this approach, the bias is equivalent to an external field and the effect of the bias is depicted by an interaction of electrons with the field. The quantum transport properties are determined by a set of occupied electron orbitals obtained by solving the time-dependent Kohn-Sham equation in Markovian process. The approach is applied to the calculation of conductance of carbon and gold wires connected to aluminum electrodes. The results are compared with available experimental and theoretical results. The current-voltage characteristic or resistance change with bias and wire sizes are also explored.

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