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Transport Through Single-Molecule Junctions: Interference, Thermopower, and the Role of Self-Interaction Effects

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Rapid progress in experiments probing transport through single molecules has opened many interesting research directions. Our theoretical work on three such directions is highlighted here; for our calculations, we combine ab initio electronic structure with a single-particle Green function description of the electronic transport. (1) We investigate the applicability of quantum interference through single molecule rings as a control mechanism in molecular electronics. We find that the quantum interference effect is strongly dependent on the interaction between molecular pi-states and contact sigma-states. Structures made with 18-annulene could be used as quantum interference effect transistors. (2) Molecular nanojunctions may support efficient thermoelectric conversion through enhanced thermopower. We calculate the thermopower for several conjugated molecular nanojunctions connected to gold electrodes. Systematic good agreement between theory and experiment is obtained– much better agreement than for comparable calculations of the conductance. (3) Finally, since we recognize that our treatment of transport is not fully justified, it is important to study corrections and extensions. We investigate the effect of the exchange-correlation potential in atomic chains by constructing optimized effective potentials using several functionals. Dramatic effects are caused by two factors: changes in the energy gap and the self-interaction error.

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