Abstract Submitted
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Quantum many-body effects on the electric and thermoelectric response of molecular heterojunctions JUSTIN BERGFIELD, CHARLES STAFFORD, University of Arizona — A semi-empirical π-electron Hamiltonian (extended Hubbard model) is used to model the electronic degrees of freedom most relevant for transport in a heterojunction consisting of a conjugated organic molecule coupled to two (or more) metallic electrodes. With an appropriate choice of parameters, the *complete spectrum of electronic excitations* of the molecule up to 8–10eV can be accurately described,[1] which is essential to accurately model transport far from equilibrium. The electric and thermoelectric response of the junction is calculated within a many-body theory of transport based on nonequilibrium Green's functions. For benzenedithiol-Au junctions, the parameters characterizing the lead-molecule coupling (tunneling width and chemical potential offset) are determined by comparison to linear-response measurements of conductance and thermopower. The nonlinear transport can then be predicted: the differential conductance as a function of gate and bias voltages exhibits clear signatures of charge quantization and resonant tunneling through excited states, with an irregular "molecular diamond" structure analogous to the regular Coulomb diamonds observed in quantum dot transport experiments. Several other small conjugated organic molecules are also investigated. [1]C. W. M. Castelton and W. Barford, J. Chem. Phys. **117**, 3570 (2002).

Charles Stafford
University of Arizona

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