Abstract Submitted
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Many-body treatment of quantum transport through single molecules JUSTIN BERGFIELD, CHARLES STAFFORD, University of Arizona
— We investigate multi-terminal quantum transport through single molecules including intramolecular correlations exactly by using the nonequilibrium Green function approach, but treating the lead-molecule coupling perturbatively via a Dyson expansion [1], with an extended Pariser–Parr–Pople molecular model. As a validation of the theory we calculate the linear and non-linear transport properties of 1,4-Benzenedithiol(BDT) and compare these results to experiment[2]. We find many transport features which are not accessible via meanfield approaches such as Coulomb Blockade steps and an incipient Hubbard-Mott insulator gap. We also calculated the thermopower exactly and find, in accordance with recent experimental[3] and theoretical reports, that the transport in this junction is dominated by holes (p-type). This result allowed us to then extract the remaining free parameter, the lead-molecule coupling Γ. The resulting nonlinear I-V curve was found to be in good quantitative agreement with experiment. Finally, we calculated the differential conductance as a function of gating and bias potential to construct a full molecular 'Coulomb diamond'.

[1]Cardamone D. et al. Nano Lett. Vol 6 2422, 2006
[2]Xiao X. et al. Nano Lett. Vol 4 267, 2004
[3]Reddy P. et al. Science. Vol 315 1568, 2007

Justin Bergfield
University of Arizona

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