Abstract Submitted
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First-Principles Studies of Aromatic Single-Molecule Junctions: Length Dependence of Conductance and Thermopower[1] SU YING QUEK, Molecular Foundry, LBNL, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University, Seoul, STEVEN G. LOUIE, Department of Physics, University of California, Berkeley; Molecular Foundry, LBNL, J. B. NEATON, Molecular Foundry, LBNL — Using a scattering-state approach incorporating self-energy corrections to the junction level alignment, the conductance G and thermopower S of oligophenyldiamine-Au junctions are calculated and elucidated. In agreement with experiment, we find G decays exponentially with the number of phenyls N with decay constant beta = 1.7. A parameter-free self-energy correction, going beyond density functional theory (DFT), is found to be essential for understanding the measured values of both G and beta (Quek et al, Nano Lett 9, 3949 (2009)). The thermopower is found to be sensitive to contact geometry. However, for each contact geometry, S increases linearly with N as found in experiment. DFT overestimates both S and the slope of S versus N, while the self-energy corrections bring both into much better agreement with experiment.

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