Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Correlated transport in molecular junctions with novel contact configurations CHARLES STAFFORD, JUSTIN BERGFIELD, JOSHUA BARR, University of Arizona — The effect on quantum transport of the geometry and connectivity of single-molecule junctions is investigated using a many-body nonequilibrium Green's function approach.[1] The variation of intramolecular interactions due to changes in screening over an ensemble of contact geometries is found to lead to significant variations of the linear transport coefficients of the junction. The transmission phase(s) and their evolution as a function of energy are found to depend strongly on the connectivity of the junction, despite being constrained by the Friedel sum-rule. For multi-channel junctions, the channel transmissions are found to deviate significantly from the predictions of mean-field approaches due to strong Coulomb correlations.

[1]J. P. Bergfield and C. A. Stafford, Phys. Rev. B **79**, 245125 (2009).

Charles Stafford
University of Arizona

Date submitted: 19 Nov 2009 Electronic form version 1.4