Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Electron correlations in transport through molecular junctions: Coulomb blockade and hysteresis in the I-V characteristics of a model system. CATALIN D. SPATARU, Columbia University, MARK S. HYBERTSEN, Brookhaven National Lab, ANDREW MILLIS, Columbia University, STEVEN G. LOUIE, University of California at Berkeley — Electron-electron interaction effects can play a very important role in explaining the mechanism of charge transport in molecular junctions. We use a simple tight-binding model to describe the leads and the electron-ion interaction inside the molecule. The electron-electron interaction inside the molecule is treated at the Hartree-Fock level. We study the model as a function of the number of sites in the molecule and the alignment of molecular energy levels relative to the average chemical potential in the leads. This model captures important phenomena such as the Coulomb blockade. We find that depending on the gate voltage and applied bias, there can be more than one Hartree-Fock steady-state solution for the system, which may give rise to a hysteresis in the I-V characteristics.

Catalin D. Spataru
Columbia University

Date submitted: 17 Nov 2006 Electronic form version 1.4