Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

End-group Influence on the Frontier Molecular Orbital Reorganization in Molecular Junctions — Effect on Thermopower JANAKIRAMAN BALACHANDRAN, Graduate Student, University of Michigan, Ann Arbor, MI, PRAMOD REDDY, Associate Professor, University of Michigan, Ann Arbor, MI, BARRY DUNIETZ, Assistant Professor, Kent State University, Kent, OH, VIKRAM GAVINI, Associate Professor, University of Michigan, Ann Arbor, MI
— The frontier molecular orbital (FMO) reorganization and in turn on the thermopower of the aromatic molecules trapped between metal electrodes (aka molecular junctions) depends on two effects namely (1) the stabilization effect – due to the physical presence of the metal electrode atoms and (2) change in e-e interactions – due to end-group mediated charge transfer. The stabilization effect always reduces the FMO energies. The charge transfer effect increases the FMO energies in charge-gaining molecules, which in turn opposes the stabilization effect resulting in a small overall shift. However, the charge transfer effect decreases the FMO energies in charge-losing molecules, which in turn complements the stabilization effect resulting in a large overall downward shift. This hypothesis is validated by delineating the shifts due to stabilization and charge-transfer effects independently. Further we also demonstrate the generality of the hypothesis by applying it on a wide range of aromatic molecules with different length and end-groups. Finally, we also present computationally efficient strategies, based on the proposed mechanism, to quantitatively compute the FMO reorganization which in turn has potential for high throughput analysis of molecular junctions.

Janakiraman Balachandran
Graduate Student, University of Michigan, Ann Arbor.

Date submitted: 15 Nov 2013 Electronic form version 1.4