Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Length dependence of conductance and thermopower of hybrid alkyl-thiophene single molecule junctions[1] MICHELE KOTIUGA, Molecular Foundry, LBNL, Department of Physics, UC Berkeley, WILLIAM B. CHANG, Department of Chemical and Biomolecular Engineering, UC Berkeley, CHENG-KANG MAI, Center for Polymers and Organic Solids, Departments of Chemistry & Biochemistry and Materials, UCSB, FABIAN PAULY, Department of Physics, Uni. Konstanz, GUILLERMO C. BAZAN, Center for Polymers and Organic Solids, Departments of Chemistry & Biochemistry and Materials, UCSB, RACHEL A. SEGALMAN, Department of Chemical and Biomolecular Engineering, UC Berkeley, JEFFREY B. NEATON, Molecular Foundry, LBNL, Department of Physics, UC Berkeley — Single-molecule junctions are novel, controllable testbeds for understanding mixed electronic and thermal transport at interfaces. Here, we study a set of newly-synthesized molecules containing alkyl and thiophene units of increasing length in order to control junction level alignment and electronic coupling with a combination of theory and experiment. Using a first-principles scattering-state approach, based on self-energy corrected density functional theory, we calculate the conductance and thermopower of thiol-terminated alkyl-thiophene-Au junctions, elucidating the relationship between length and thermopower. We compare our work to statistical measurements with a scanning tunneling microscope-based break junction technique, and discuss the impact of junction geometry on our results.

[1]Work supported by ONR/AFOSR BAA 10-026 and computational resources provided by NERSC.

Michele Kotiuga
Molecular Foundry, LBNL, Department of Physics, UC Berkeley

Date submitted: 14 Nov 2013 Electronic form version 1.4