

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Tailoring IV Characteristics and Rectification in Single-Molecule Junctions¹ PIERRE DARANCET, Lawrence Berkeley National Laboratory, JONATHAN WIDAWSKY, Columbia University, HYOUNG JOON CHOI, Yonsei University, LATHA VENKATARAMAN, Columbia University, JEFFREY NEATON, Lawrence Berkeley National Laboratory — Asymmetry in the current-voltage characteristics, or current rectification, of nanoscale junctions is a critical property for many optoelectronic and energy conversion applications using nanostructured materials. Here, we compute the conductance, IV characteristics, and bias-dependent rectification of a class of molecular junctions, consisting of donor-acceptor molecules in contact with Au electrodes, using quantitative first-principles calculations [1]. We relate the rectification to the identities of the donor and acceptor moieties through the junction energy level alignment and dipole moments and find, surprisingly, that a large asymmetry in the contact coupling leads to weak rectification. We explain our results with an analytic coherent tunneling model, and suggest concrete strategies for obtaining high rectification in experimentally-achievable systems. [1] Darancet et al. , submitted (2011) .

¹We acknowledge DOE-BES for support and NERSC for computational resources.

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Date submitted: 11 Nov 2011

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