Abstract Submitted
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Ab initio studies of electronic transport through amine-Au-linked junctions of photoactive molecules[1] DAVID A. STRUBBE, Dept. of Physics, University of California, Berkeley; Materials Sciences Division, Lawrence Berkeley National Laboratory, SU YING QUEK, Molecular Foundry, LBNL, LATHA VENKATARAMAN, Dept. of Applied Physics, Columbia Univ., HYOUNG JOON CHOI, Dept. of Physics and IPAP, Yonsei Univ., J.B. NEATON, Molecular Foundry, LBNL, STEVEN G. LOUIE, Dept. of Physics, UC Berkeley; MSD, LBNL — Molecules linked to Au electrodes via amine groups have been shown to result in reproducible molecular conductance values for a wide range of single-molecule junctions [1,2]. Recent calculations have shown that these linkages result in a junction conductance relatively insensitive to atomic structure [3]. Here we exploit these well-defined linkages to study the effect of isomerization on conductance for the photoactive molecule 4,4'-diaminoazobenzene. We use a first-principles scattering-state method based on density-functional theory to explore structure and transport properties of the cis and trans isomers of the molecule, and we discuss implications for experiment. [1] L Venkataraman et al., Nature 442, 904-907 (2006); [2] L Venkataraman et al., Nano Lett. 6, 458-462 (2006); [3] SY Quek et al., Nano Lett. 7, 3477-3482 (2007).

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