Abstract Submitted
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First-principles Studies of Single-molecule Conductance in Amine Linked Junctions[1] SU YING QUEK, The Molecular Foundry, Lawrence Berkeley National Lab, MARK S. HYBERTSEN, Center for Functional Nanomaterials, Brookhaven National Lab and Columbia University, LATHA VENKATARAMAN, Physics Department, Columbia University, MICHAEL STEIGERWALD, COLIN NUCKOLLS, Chemistry Department, Columbia University, STEVEN G. LOUIE, Physics Department, University of California, Berkeley and Lawrence Berkeley National Lab, J.B. NEATON, The Molecular Foundry, Lawrence Berkeley National Lab — Recently, it was discovered that the conductance of single molecule junctions with amine linkages to Au electrodes can be reliably and reproducibly measured. We compute and examine the conductance of prototypical single molecule junctions formed with amine-Au links using a first-principles scattering state method based on density functional theory. In particular, we elucidate the nature of the scattering states that give rise to the computed conductance, and relate the transmission spectra of each junction to intrinsic molecular and amine link properties. We explore the sensitivity of our results to specific contact geometries. The results are discussed relative to the measured distribution of conductance for each molecule.

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