

Abstract Submitted
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Theory of Solvent-Mediated Environmental Effects on Molecular-Scale Transport MICHELE KOTIUGA, Department of Physics, UC Berkeley & Molecular Foundry, LBNL, PIERRE DARANCET, Molecular Foundry, LBNL, VALLA FATEMI, Department of Physics, MIT, BIRGER HENNINGS, MICHAEL FREI, LATHA VENKATARAMAN, Department of Applied Physics and Applied Mathematics, Columbia, JEFFREY NEATON, Molecular Foundry, LBNL — Single-molecule junctions, formed with well-defined and robust metal-molecule contacts, can provide an ideal model system to study mechanisms of charge transport at the molecular scale. However, the presence of solvent is often unavoidable, and recent experiments have shown that the junction conductance can be altered by a factor of two depending on the solvent present [1]. It has been proposed that the binding of the solvent to the gold electrodes changes their local work function, which in turn alters the conductance of the junction in a predictable manner. Here, we use a first-principles scattering-state approach, based on self-energy corrected density functional theory, to explore the transmission and conductance of bipyridine- and diaminestilbene-Au molecular junctions in the presence of solvent molecules, using an analytical model to compare with experimental results. We acknowledge DOE for support, and NERSC for computational resources.

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