Theory of Solvent Effects on Charge Transport in Molecular Junctions

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Abstract: Experimentally, it has been observed that changing the solvent can alter the conductance of a molecular junction by up to a factor of two [2] or more. Here, we elucidate the effect of solvent on molecular junction transport properties and show how ab initio density functional theory calculations of conductance can be extended to incorporate solvent effects, unavoidable in any STM break junction experiment. We explain shifts in conductance associated with solvent as a local gating effect caused by solvent molecules bound to surfaces near the junction. We demonstrate this via ab initio self-energy corrected [1] transmission calculations of 4,4'-bipyridine on gold in which various molecular coverages results in a shift in the local potential of the junction, altering the junction energy level alignment and enhancing the conductance by more that a factor of 50%. Furthermore, we develop a general electrostatic model, incorporating experimental parameters, system thermodynamics, and first-principles calculations, that elucidates the relationship between molecular adsorption and the junction potential and conductance [3].

[1]Nano Lett. 9, 3949-3953, 2009
[2]Nano Lett. 11, 1988-1992, 2011
[3]Kotiuga, M., et. al., ArXiv cond-mat.mes-hall/1410.1439