Abstract Submitted
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Theoretical Analysis of the Trends in Single Molecule Junction Conductance Formed Using Amine-Gold Links[1] MARK HYBERTSEN, Brookhaven National Laboratory, MICHAEL STEIGERWALD, LATHA VENKATARAMAN, COLIN NUCKOLLS, Columbia University — The conductance of single molecule junctions using amine-gold links has now been measured for several families of molecules. Systematic trends are revealed with length, conjugation, conformation and substituents. The amine link group binds to undercoordinated gold atoms in the junction through a donor- acceptor type bond. The frontier orbitals that result are consistent with flexible and reproducible electronic coupling between the electrodes and the molecules. A simple proxy for the Au link site in each electrode allows direct calculation of the tunnel coupling through the molecule. The calculated trends in tunnel coupling are in excellent agreement with experiment within each family studied. Surprisingly, the trends between different families are also reproduced, albeit with a modest offset between families. The comparison between families is proposed to also involve small changes in the alignment of the gateway states controlling tunnel coupling with the electrode Fermi Energy.

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