

Abstract Submitted
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Theoretical Exploration of the Impact of Link Chemistry on Single Molecule Junction Conductance¹ MARK S. HYBERTSEN, Applied Physics and Applied Math. Dept, Columbia University, MICHAEL STEIGEWALD, Chemistry Dept., Columbia University, LATHA VENKATARAMAN, Physics Dept., Columbia University, JENNIFER E. KLARE, IRIS W. TAM, COLIN NUCKOLLS, Chemistry Dept., Columbia University — Measurement of molecular conductance by repeatedly breaking an Au point contact in an environment of molecules allows for the study of a large number of fresh junctions and presents a statistical picture of the junction conductance. However, there is no direct control or knowledge of the atomic scale structure in each individual junction. It is important to distinguish effects on the conductance related to the structure of the metal-molecule link from those that are intrinsic to the backbone of the molecule in the junction. To that end, we examine the energetics and frontier electronic states of various link groups such as thiolate and isonitrile coupled to candidate Au structures using DFT based calculations. We discuss systematic trends in comparison with experiments.

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Mark S. Hybertsen
Applied Physics and Applied Math. Dept, Columbia University

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