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Conductance of Single Molecule Junctions: Dependence on Structure and Conformation¹

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We recently demonstrated that the conductance of single molecule junctions formed by breaking Au point contacts in an environment of molecules with amine linkages can be measured reliably and reproducibly¹. We have now studied junctions formed by approximately 30 different amine terminated molecules, allowing systematic study of the correlation between molecular properties and single molecule junction conductance. This talk will focus on the relation between molecular conductance and molecule conformation for the simple case of a biphenyl, two benzene rings linked together by a single C-C bond. Our results from a series of seven biphenyl derivatives show that the molecular junction conductance depends on the twist angle. Specifically, we find that the planar molecule has the highest conductance, and the conductance for the series decreases with increasing twist angle, consistent with a cosine squared relation predicted theoretically². 1. L. Venkataraman, J.E. Klare, I.W. Tam, C. Nuckolls, M.S Hybertsen and M. Steigerwald, *Nano Letters*, vol. 5, pp. 458-462, 2006. 2. L. Venkataraman, J.E. Klare, C. Nuckolls, M.S Hybertsen and M. Steigerwald, *Nature*, vol. 442, pp. 904-907, 2006.

¹NSF Nanoscale Science and Engineering Center at Columbia University and New York State Office of Science (NYSTAR)