# Simultaneous Measurements of Force and Conductance in Single-Molecule Circuits

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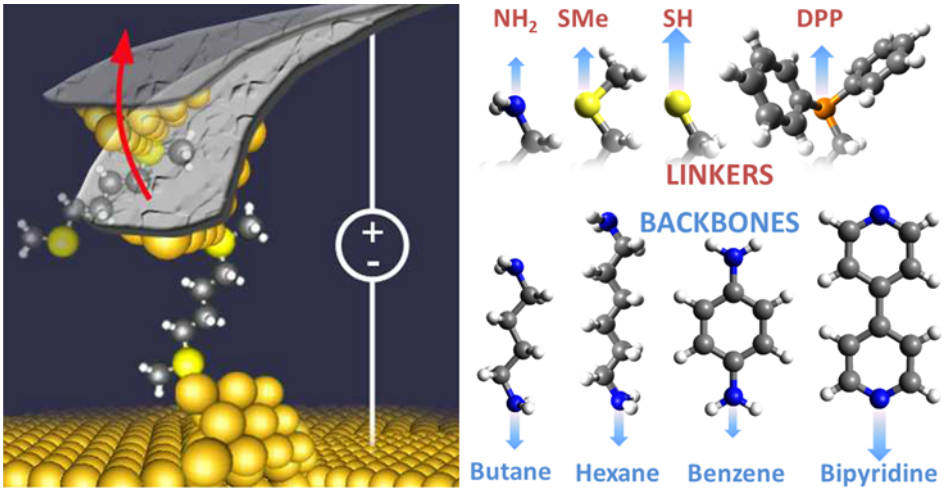
Probing the relation between mechanical and electronic properties of single molecule circuits provides a deeper understanding of the structure-conductance relation in these systems. In this talk, I will present experimental techniques used to measure these properties in single-molecule circuits using a custom-built conducting atomic force microscope [1]. With this set-up, we can simultaneously measure conductance and force across single Au-molecule-Au junctions in order to obtain complementary information about the electronics and structure in these systems. We find that single-atom Au contacts, which have a conductance of $G_0$ ($2e^2/h$), have a rupture force of about 1.5 nN, in excellent agreement with previous theoretical and experimental studies. For a series of amine and pyridine linked molecules, which are bound to Au electrodes through an Au-N donor-acceptor bond, we find that the rupture force depends on the backbone chemistry and can range from 0.5 nN to 0.8 nN [1]. We also study junctions formed with molecules that bind through P-Au and S-Au interactions. We find that both the conductance signatures and junction evolution of covalent S-Au bond (thiolate) and a donor-acceptor S-Au bond (thiol) are dramatically different [2]. Finally, I will show how the simultaneous measurements of forces can be used to demonstrate effects related to quantum interference in single-molecule junctions [3].




**References**

[1] M. Frei, S. V. Aradhya, M. Koentopp, M. S. Hybertsen, and L. Venkataraman, "Mechanics and Chemistry: Single Molecule Bond Rupture Forces Correlate with Molecular Backbone Structure", *Nano Lett.* **11**, 1518-1523 (2011).

[2] M. Frei, S. V. Aradhya, M. S. Hybertsen, and L. Venkataraman, "Linker Dependent Bond Rupture Force Measurements in Single-Molecule Junctions", *J. Am. Chem. Soc.* **134**, 4003-4006 (2012).

[3] S. V. Aradhya, J. S. Meisner, M. Krikorian, S. Ahn, R. Parameswaran, M. L. Steigerwald, C. Nuckolls, and L. Venkataraman, "Dissecting Contact Mechanics from Quantum Interference in Single-Molecule Junctions of Stilbene Derivatives", *Nano Lett.* **12**, 1643-1647 (2012).