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Single Molecule Junctions: A Laboratory for Chemistry, Mechanics and Bond Rupture

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Invited Presentation
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Abstract

Simultaneous measurement [1] of junction conductance and sustained force in single molecule junctions bridging metal electrodes provides a powerful tool in the quantitative study of the character of molecule-metal bonds. In this talk I will discuss three topics. First, I will describe chemical trends in link bond strength based on experiments and Density Functional Theory based calculations. Second, I will focus on the specific case of pyridine-linked junctions. Bond rupture from the high conductance junction structure shows a requires a force that exceeds the rupture force of gold point contacts and clearly indicates the role of additional forces, beyond the specific N-Au donor acceptor bond. DFT-D2 calculations with empirical addition of dispersion interactions illustrates the interplay between the donor-acceptor bonding and the non-specific van der Waals interactions between the pyridine rings and Au asperities. Third, I will describe recent efforts to characterize the diversity of junction structures realized in break-junction experiments with suitable models for the potential surfaces that are observed.

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