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**Mechanical control of frontier orbital alignment in single molecule junctions** CHRIS BRUOT, Arizona State University, JOSHUA HIHATH, University of California - Davis, NONGJIAN TAO, Arizona State University — The unique interplay between electronic and mechanical properties of molecular electronic systems offers opportunities to create novel devices and investigate new phenomena not seen in conventional electronics. Here we will discuss the electromechanical properties of a simple molecular system, a single 1,4-benzenedithiol (BDT) molecule bound to the Au electrodes of a STM, which display a counterintuitive increase in conductance when stretched [1]. This conductance behavior is attributed to the coupling of frontier molecular orbitals with the electrodes. By stretching and compressing BDT molecular junctions we are able to show that weakening of the coupling between molecule and electrode causes the energy of the frontier orbital to approach that of the Fermi level, moving the transport towards resonance. This effect is measured experimentally by recording conductance vs. stretching distance trace for single molecule junctions. Additionally, conductance-voltage and IETS spectra indicate that stretching and compressing a single BDT junction causes reversible change in the molecule-electrode coupling. Finally, transition voltage spectroscopy shows the change in energy of the frontier orbital as a single molecule junction is stretched. The measured behavior of BDT is a consequence of the molecular scale interactions that dominate mesoscopic transport and set molecular electronics apart from conventional electronics.

[1] C. Bruot, J. Hihath, and N. Tao, Nature Nanotechnology 7, 35 (2012).

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