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Correlating Molecular Energy Level Alignment with the Conductance of Single Molecular Junctions TAEKYEONG KIM, JONATHAN R. WIDAWSKY, Columbia University, PIERRE DARANCET, MICHELE KOTIUGA, JEFFREY B. NEATON, Lawrence Berkeley National Laboratory, LATHA VENKATARAMAN, Columbia University — There has been increased interest in understanding electronic and thermoelectric transport in single molecule junctions and metal/organic interfaces. While the ionization potential and electron affinity of molecules can be calculated for molecules in the gas-phase, additional physical effects, such as charge transfer and rearrangement, hybridization, and electrode polarization are expected to alter these electronic energies for molecular junctions. Therefore, it is hard to determine energy level alignments in molecular junctions. Here, we determine the relationship between electronic energy level alignment at a metal-molecule-metal interface and single-molecule junction conductance properties for 4,4'-bipyridine via direct and simultaneous measurement of electrical and thermoelectric currents using a scanning tunneling microscope-based break-junction technique. We measure directly, the position of the lowest unoccupied molecular orbital (LUMO) relative to the Au Fermi level assuming a Lorentzian resonance lineshape. Furthermore, we correlate the energy level alignment and coupling strength between two conductance states through repeated junction elongation and compression. We find that these values are in excellent agreement with our self-energy corrected density functional theory calculations. These results thus provide the first evidence for correlation between energy level alignment and single molecule transport.

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