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Revealing Transmission in Metal-Molecule Junctions Using Length Dependant Thermopower Measurements JONATHAN A. MALEN, PETER DOAK, KANHAYALAL BAHETI, T. DON TILLEY, ARUN MAJUMDAR, RACHEL A. SEGALMAN, UC Berkeley — Conductance in metal-molecule junctions is known to trend with molecular endgroups, backbone, and length, but a more complete picture of the junction's transmission structure has been hitherto elusive. We now report complimentary trends in the junction's thermopower (S) that reveal length dependent changes in molecular orbital alignment and coupling with contact states. Phenylenediamines, phenylenedithiols, and alkanedithiols trapped between gold contacts were examined. S increases linearly with length for phenylenediames and dithiols while it decreases linearly in alkanedithiols. Comparison of this data suggests that the molecular backbone determines the length dependence of S, while the endgroup determines the zero-length, or contact S. Transport in phenylenes was dominated by the HOMO, which moves closer to the Fermi energy of the contacts as $\sim 1/L$, and broadens due to contact coupling as $\sim e^{-L}$. In contrast, the decreasing trend in S for alkanedithiols suggests that transmission is largely effected by gold-thiol gap states between the HOMO and LUMO.

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