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Effects of Molecule-Electrode Binding on Molecular Junctions PETER DOAK, Chemistry UC Berkeley, JON MALEN, Mech. Eng, UC Berkeley, KANHAYALAL BAHETI, Chemistry UC Berkeley, ARUN MAJUMDAR, Mech. Eng, UC Berkeley, RACHEL SEGALMAN, Chem. Eng. UC Berkeley, DON TILLEY, Chemistry UC Berkeley — Measurements of the Seebeck coefficient or thermopower of metal-molecule-metal junctions offer additional insight into single molecule transport. By applying a temperature bias across a junction created via an Au-Au STM break junction a thermoelectric voltage can be measured which is related to the transmission function through a derivative. Previously dithiol molecules have been studied by this method. Here, the effects of altering the binding to the electrodes will be demonstrated. When the binding group is altered to cyano or amine functionalities, the thermopower is greatly affected suggesting markedly different behavior in response to tuning of molecular energy levels. This indicates important changes in the junction transmission functions near the chemical potential of the contacts. For example, we show that measurements of dinitrile molecules cannot be interpreted as simple shifts of a single Lorentzian transmission peak across the contact chemical potential. Additionally these measurements show that the binding groups can have considerably more influence on junction behavior than other forms of molecular functionalization and provide a useful means to interrogate theories of junction transport.

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