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Simultaneous Determination of Conductance and Thermopower of Single Molecule Junctions[1] JONATHAN WIDAWSKY, Department of Applied Physics and Applied Mathematics, Columbia University, PIERRE DARANCET, JEFFREY NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory, LATHA VENKATARAMAN, Department of Applied Physics and Applied Mathematics, Columbia University — We present a study of concurrent determination of conductance (G) and thermopower (S) of single-molecule junctions via direct measurement of electrical and thermoelectric currents. The junctions are created using the STM-based break-junction technique where a cold Au tip is repeatedly brought in and out of contact with a hot Au-on-mica substrate in an environment of the target molecule. We explore several amine-Au and pyridine-Au linked molecules that are predicted to conduct through either the highest occupied molecular orbital (HOMO) or the lowest unoccupied molecular orbital (LUMO), respectively. We find that the Seebeck coefficient is negative for pyridine-Au linked LUMO-conducting junctions and positive for amine-Au linked HOMO-conducting junctions. From histograms of thousands of junctions, we use the most probable Seebeck coefficient to determine a power factor, GS^2, for each junction studied, and find that GS^2generally increases with G.

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