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Tuning the Thermoelectric Properties of Metal-Molecule-Metal Junctions K. BAHETI, J.A. MALEN, P. DOAK, T.D. TILLEY, A. MAJUMDAR, R. SEGALMAN, Univ. of California, Berkeley — Thermoelectric materials have application in power generation and refrigeration, with several advantages over conventional power cycles including lack of moving parts, silent operation, miniaturization, and CO2 free conversion of heat to electricity. Nonetheless, low thermodynamic efficiency has limited their applicability. Here we examine a new class of inexpensive thermoelectric materials composed of organic-inorganic heterostructures. Thermopower measurements of 1,4-Benzenedithiol (BDT) molecule between Au electrodes, using a modified scanning tunneling microscope (STM), have been previously reported. This method is used to interrogate junctions where, the BDT molecule has been doped by the addition of substituent groups on the benzene ring. Our measurements show that we can tune the thermoelectric properties of such junctions in a controllable way by the addition of substituents. This in conjunction with a calculated transmission function imply a simultaneous increase in the thermopower and conductance, which has hitherto been impossible to attain in simple materials. We observe an increase of $\sim$50% in the power factor, defined as $S^2\sigma$, of the junction upon substitution of electron donating groups in benzenedithiol. Hence, a ground up approach to building thermoelectric materials, from an endless array of possible organic-inorganic heterostructures, evokes hope for efficient thermoelectric energy conversion.

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