Single Molecule Thermoelectricity

MSD Faculty Scientists Rachel Segalman and Arun Majumdar have discovered thermoelectricity—the conversion of heat to electricity—in devices with a single molecule sandwiched between two metal surfaces. While the amount of electricity that can be generated is, at present, small, this is a promising first example of the new field of molecular thermoelectrics.

About 90 percent of the world's power is generated by engines that convert heat to mechanical motion, which can then be converted to electricity. However, nature requires that we to pay a penalty for this process: not all of the heat can be converted to power and the resultant waste heat is released to the environment. [For example, the role of the radiator in a car to dissipate the excess engine heat.] If even a fraction of this low-grade heat could be converted to electricity in a cost-effective manner, the impact on energy consumption could be enormous, amounting to a massive savings of fuel with accompanying decrease in atmospheric carbon dioxide.

Thermoelectric energy converters exist that can directly convert low-grade heat to electricity using semiconducting materials. These devices rely on a phenomenon known as the Seebeck effect, in which a voltage is produced when a temperature differential is applied across a material. Solid-state electric power generators and refrigerators based on thermoelectrics are commercially available, but the widespread use of such devices is limited due to their low efficiency and the high cost of the materials. For example, today's thermoelectric generators operating across a temperature differential of 1000 ^{o}C on the hot side and 25 ^{o}C on the cold side have an efficiency of ~7%, while a traditional engine operating under the same conditions has an efficiency of ~ 20%. Researchers have been working for over 50 years to develop better thermoelectric materials and while some advances have been made with nanostructured materials, expensive inorganic materials and high temperature semiconductor processing are required, making their widespread use prohibitive.

Segalman and Majumdar have taken an entirely different approach. Realizing that the alignment of the electronic energy levels in materials changes when a chemical bond is formed, they hypothesized that molecules sandwiched between metals or semiconductors might have desirable thermoelectric properties. By using a modified scanning tunneling microscope (see figure) they discovered that when placed in this configuration, organic molecules such as benzenedithiol, which had not been previously considered for thermoelectric use, do indeed exhibit a Seebeck effect.

The organic molecules and metal nanoparticles involved here are inexpensive and easily processed, and thus, if efficiencies can be improved, this offers the promise of low cost plastic-like power generators and refrigerators. Further research is being carried out to tune both the metal-molecule junctions by modifying both the chemistry of the molecules and also their contact with the metal.

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Pramod Reddy, Sung-Yeon Jang, Rachel Segalman and Arun Majumdar, "Thermoelectricity in Molecular Junctions," *Science* **315**, 1568 (2007).

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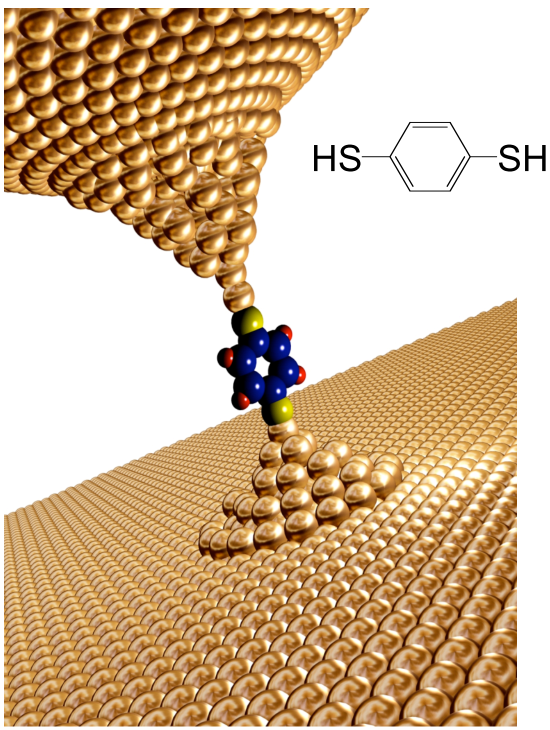
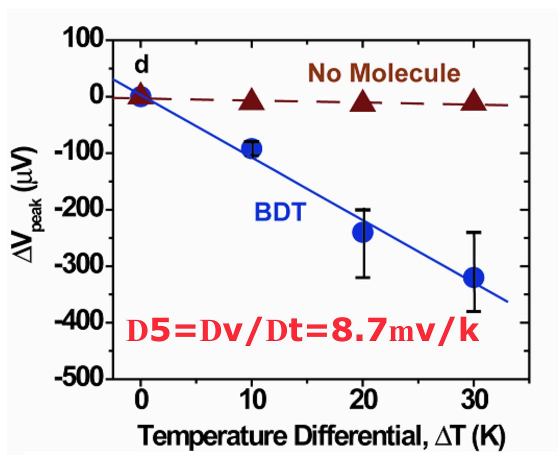
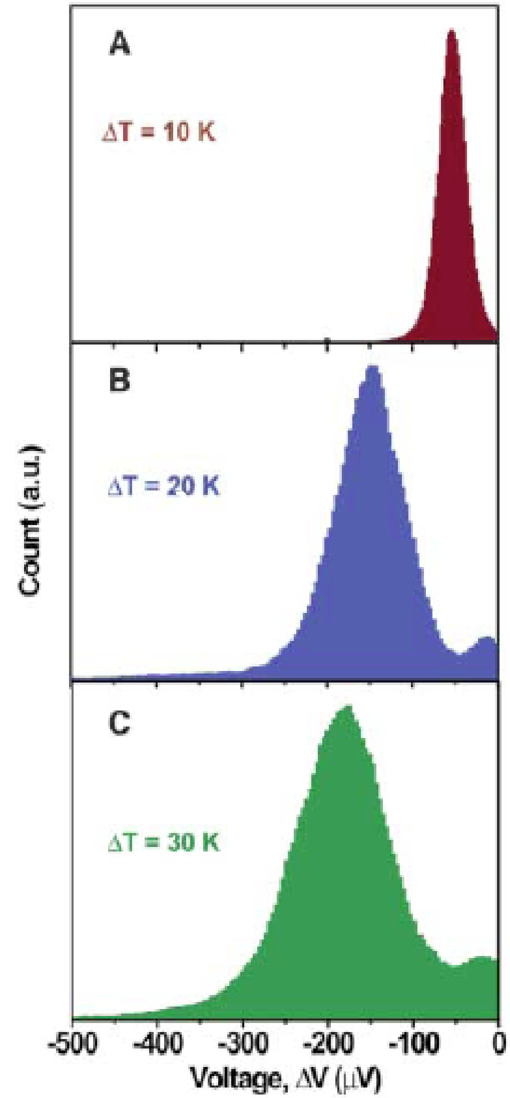
Schematic *of a single molecule of benzenedithiol suspended between the tip of a scanning tunneling microscope and a gold substrate. By heating the substrate and monitoring the voltage difference between the tip and the solvent, a thermoelectric response of a single molecule can be measured. (Bump on the gold substrate is an artifact of the contact with the STM tip.)*



Histograms *from measurements of 1000 different benzenedithiol molecules showing the thermoelectric potential generated due to the Seebeck effect as a function of the temperature difference between the tip and substrate. The measured voltage varies linearly with the temperature differential, as expected.*



Plot of the voltage *against the temperature differential of the device.*



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