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Molecular Thermoelectrics

RACHEL SEGALMAN, UC Berkeley and Lawrence Berkeley National Laboratories

Thermoelectric materials for energy generation have several advantages over conventional power cycles including lack of moving parts, silent operation, miniaturizability, and CO2 free conversion of heat to electricity. Historically, these materials suffered from low efficiency and have involved very expensive inorganic compounds. We demonstrate that some metal-molecule-metal junctions produce voltage when exposed to heat. This exciting initial demonstration of thermopower from molecular junctions is reinforced by the fact that relatively minor changes to chemical structure result in an unprecedented simultaneous increases in both thermopower and electrical conductance, suggesting that highly efficient devices may be *designed* in a manner impossible in traditional thermoelectric materials. Furthermore, thermopower measurements offer an alternative transport measurement that can characterize the dominant transport orbital and is independent of the number of molecules in the junction. In particular, the effect of substituents and endgroups on the electronic behavior of gold-1,4-benzenedithiol -gold junctions (BDT) is explored.