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**Transport properties and the thermoelectric figure-of-merit of single molecule systems.** PADRAIG MURPHY, Department of Physics, UC Berkeley, SUBROTO MUKERJEE, JOEL MOORE, Department of Physics, UC Berkeley, and Materials Sciences Division, Lawrence Berkeley National Laboratory — The thermoelectric properties of molecules are both of fundamental interest and of interest for the construction of energy conversion devices. These transport properties are sensitive to interactions within the molecule, the hybridization energy between the molecular energy levels and the leads, and to the temperature. We present numerical and theoretical results on the conductance and thermopower, and discuss the parameter values for which the figure-of-merit, which parametrizes the efficiency of energy conversion devices, is optimal. The numerical results for the thermopower can be obtained at fixed particle number for finite systems using an appropriate generalization of the approach of Gogolin and Prokof'ev to electrical conductance.

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