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Using Non-Equilibrium Green's Functions to Study Nanoscale Thermoelectricity ARUNIMA COOMAR, CHARLES STAFFORD, University of Arizona — The Green's function is a concept that gives us the response at any point inside or outside a conductor due to an applied excitation at any other. The nonequilibrium Green's Function (NEGF) formalism (aka the Keldysh formalism) is a powerful tool that provides a microscopic theory for interacting quantum systems out of equilibrium. In this poster, we demonstrate the use of the Keldysh approach to predict and calculate thermoelectric quantities such as the Thermopower (S) and the dimensionless figure of merit (ZT) across a single-molecule junction (SMJ). We show that it is possible to get very large thermoelectric effects in SMJs with cross-conjugated molecules, which exhibit destructive quantum interference of the electron waves. These studies are potentially useful in the development of efficient thermoelectric devices to constitute a commercially viable solution for many heating and cooling problems at both the macro and nanoscale, with no operational carbon footprint.

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