

Abstract Submitted
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Tuning nanoscale thermoelectricity with electron-electron interactions¹ ARUNIMA COOMAR, CHARLES STAFFORD, University of Arizona — The Nonequilibrium Green's Function (NEGF) formalism is a powerful tool that provides a microscopic theory for interacting quantum systems out of equilibrium. In this talk, I will be presenting a few results obtained using the NEGF approach combined with pi-electron effective field theory to study the thermoelectric transport properties such as the thermopower (S) and the dimensionless figure of merit (ZT) across single-molecule junctions with pi-conjugated molecular systems, which exhibit destructive quantum interference of the electron waves. Some interesting results showcasing the tuning of the thermoelectric properties by embedding the junctions in a dielectric medium will be presented, along with our ongoing investigations of the transmission node spectrum in these molecular junctions, and the enhanced thermoelectricity resulting from it.

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