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Nonlinearities and Noise Properties of Electronic Heat Transfer in Molecular Junctions[1] ARTHUR LUNIEWSKI, RITA AGHJAYAN, KAMIL WALCZAK, Department of Chemistry and Physical Sciences, Pace University, 1 Pace Plaza, New York City, NY 10038, NANOSCALE PHYSICS DIVISION TEAM
— We examine the electronic heat transport phenomena in nanoscale junctions composed of organic molecules weakly coupled to two heat reservoirs of different temperatures. The electronic heat flux and its dynamical noise properties are calculated within the scattering (Landauer) formalism with the transmission probability determined by using non-equilibrium Green's functions technique. The perturbative computational scheme is used to determine nonlinear corrections to the electronic heat flux and its noise power spectral density with up to the second order terms in relation to the temperature difference. Our results show the limited applicability of ballistic Fourier's law and the fluctuation-dissipation relations to nanoscale heat flow carried by electrons. Further, we discuss the influence of quantum interference and dimensionality of heat reservoirs onto the transport characteristics and shot noise spectra related to molecular systems under consideration. Importantly, the nonlinear transport theory developed by us may be extended to higher order terms to address a huge variety of problems associated with nonlinear thermal effects, which may occur at nanoscale.

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