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Inelastic Heat Transfer in Molecular Quantum Dots JOANNA DYRKACZ, KAMIL WALCZAK, Pace Univ — We examine electronic heat conduction via molecular complexes in the presence of local electron-phonon coupling effects. In off-resonance transport regime, even weak electron-phonon interactions lead to phonon-mediated changes of transport characteristics. In the nearly resonance conditions, the strong electron-phonon coupling reduces the height of the main conductance peak, generating additional satellites (phonon sidebands) in transport characteristics and shifting molecular energy spectrum via reorganization (polaron) energy. In the past, it was shown that inclusion of electron-phonon coupling effects into computational scheme reduces discrepancy between theoretical results and experimental data. The aim of this project is to study electron-phonon coupling effects on electronic heat transfer at molecular level. For that purpose, we use non-perturbative computational scheme based on inelastic version of Landauer formula, where the Green's functions technique combined with polaron transformation was used to calculate multi-channel transmission probability function, while accessibility of individual conduction channels is governed by Boltzmann statistics. Our analysis is based on the hypothesis that the dynamics created by electron-phonon interaction onto the molecular quantum dot asymmetrically connected to two thermal reservoirs will lead to thermal rectification effect. Our results will be discussed in a few aspects: electron-phonon coupling strength, phonon dispersion relationship, and heat fluxes generated by temperature difference as well as bias voltage.

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