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Electron-Phonon Coupling Effects in Molecular Heat Conduction JOANNA DYRKACZ, KAMIL WALCZAK, Pace University — We examine electronic heat conduction via molecular complexes in the presence of local electron-phonon coupling effects. Specifically, we analyze transport characteristics of molecular junction regarding the strength of molecule-reservoir and electron-phonon coupling parameters, temperature and energy of molecular vibrations. We also perform a detailed analysis of the influence of phonon-assisted processes and the structure of phonon sidebands onto heat fluxes. 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 molecule asymmetrically connected to two thermal reservoirs will lead to thermal rectification effect.

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