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The impact of electron-vibration interactions on the thermoelectric efficiency of molecular junctions BAILEY HSU, JI-WEI JIANG, YU-CHANG CHEN, Department of Electrophysics, National Chiao-Tung University — From first–principles approaches, we investigate the thermoelectric efficiency of a molecular junction where a benzene molecule is connected directly to the platinum electrodes. We calculate thermoelectric figure of merits ZT in the presence of electron–vibration interactions with and without local heating under two scenarios: linear response (zero bias) and finite bias (non–zero bias) regimes. In the linear response regime, ZT saturates around the electrode temperature $T_e = 25$ K in the elastic case, while in the inelastic case we observe a non–saturated and a much larger ZT beyond $T_e = 25$ K attributed to the tail of the Fermi–Dirac distribution. In the finite bias regime, the inelastic effects reveal the signatures of the molecular vibrations in the low temperature regime. The normal modes exhibiting structures in the inelastic profile are characterized by large components of atomic vibrations along the current density direction on top of each individual atom. In all cases, the inclusion of local heating leads to a higher wire temperature T_w and thus magnifies further the influence of the electron–vibration interactions due to the increased number of local phonons.

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