Deformation potential approximation to evaluating the thermoelectric figure of merit for molecular materials

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Abstract

We propose a combined computational scheme to predict the thermoelectric properties of organic semiconductors, taking α-form phthalocyanine crystals H_2Pc, CuPc, NiPc, and TiOPc as examples. This completely parameter-free approach combines first-principles band structure calculations, Boltzmann transport theory, deformation potential theory for electron-phonon coupling, and the non-equilibrium molecular dynamics for heat transport. We abandon the constant relaxation time approximation commonly practiced in literature. Instead, we calculate it from first-principles with the deformation potential approximation. The obtained Seebeck coefficients are in good agreement with experiment, validating our treatment for relaxation time. From the calculated thermoelectric figure of merit (ZT) value, we show that phthalocyanine crystals could be excellent thermoelectric materials when n-doped, with the highest ZT value of 2.5 in NiPc at the doping level of -1.5×10^{20} cm^{-3}.