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Thermoelectric properties improvement in quasi-one-dimensional organic crystals

ABSTRACT

The charge and energy transport in highly conducting quasi-one-dimensional organic crystals of p-type tetrathiotetracene-iodide, TTT2I3, and of n-type tetrathiotetracene-tetracyanoquinodimethane, TTT(TCNQ)2, is studied. Two electron-phonon interactions are considered simultaneously. One interaction is of the acoustic deformation potential type and the other one is of polaronic character. Charge transport along the conducting molecular chains is bandlike, whereas in the transversal directions, it is of the hopping type. It is shown that due to a partial compensation of these interactions for a narrow interval of states in the one-dimensional conduction band, the relaxation time is of Lorentzian shape and shows a distinct dependence on carrier energy with a pronounced maximum. The scattering of charge carriers on adjacent molecular chains and by impurities and structural defects limits the height of this maximum. However, rather high relaxation times might be anticipated in the case of

perfect single crystals. As the carriers in these states show an enhanced mobility, this will lead to a simultaneous increase of electrical conductivity and Seebeck coefficient. It is proposed that, if the above-mentioned crystals could be accomplished by means of sufficient purification and by optimization of the carrier concentration, so that the Fermi level is close to energetic states for which the relaxation time has a maximum, one might achieve values for the thermoelectric figure of merit ZT~5 in crystals of tetrathiotetracene-iodide and ZT~1.5 in those of tetrathiotetracene-tetracyanoquinodimethane.