Contributed Talk

Promising Organic Thermoelectric Material of n-Type

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In the last years, organic materials attract more and more attention for thermoelectric applications as materials with more diverse properties, accessible row components and obtained by cost-effective environmentally friendly production technology. Usually, the materials of *n*-type have lower values of the thermoelectric figure of merit *ZT*, then those of *p*-type. Therefore, it is important to search materials of *n*-type with improved thermoelectric performance. In this paper, the thermoelectric properties of *n*-type organic crystals of tetrathiotetracene-tetracyanoquinodimethane, $TTT(TCNQ)_2$, are modeled in addition to [1]. The most complete 3D physical model is applied, which takes into account two the most important electron-phonon interactions. One interaction is of

deformation potential type and the other is similar to that of polaron. The electron-impurity interaction is considered as well. The expected values of the thermoelectric figure of merit are determined for crystals with different degrees of perfection and carrier concentration. Optimal values of electrical conductivity, Seebeck coefficient, and electronic thermal conductivity in order to achieve optimal values of the thermoelectric figure of merit are calculated. It is shown that in order to increase the thermoelectric figure of merit in this material it is necessary to increase the concentration of conduction electrons and to improve the crystal purity and perfection. It is obtained that, if the carrier concentration is increased by two times with respect to stoichiometric one and the crystals are further purified, values of $ZT \sim 1.2$ are expected, higher than reported until now.

[1] Sanduleac I., Casian A., Nanostructured $TTT(TCNQ)_2$ Organic Crystals as Promising Thermoelectric *n*-Type Materials: 3D Modeling, *Journal of Electronic Materials*, **45**(3), pp. 1316–1320, 2015. https://doi.org/10.1007/s11664-015-4018-8