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Low-Dimensional Organic Crystal Tetrathiotetracene–Iodide as Thermoelectric Material: Reality and Prospects

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Abstract

It is explained the strong dependence of electrical conductivity and very weak dependence of thermopower on crystal purity observed experimentally in ordinary quasi-one-dimensional organic crystals of tetrathiotetracene–iodide, TTT_2I_3 . It is shown theoretically that in really existing crystals TTT_2I_3 it is possibly to increase the dimensionless thermoelectric figure of merit ZT up to 1.4 at room temperature, if the carriers concentration is diminished by approximately 2.5 times with respect to the concentration in stoichiometric crystals. For purer crystals with a slightly less impurity concentration values of $ZT \sim 2$ are expected. Whole predicted increase of ZT is expected as a result of the thermoelectric power factor growth.