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Peierls Structural Transition in Q1D Crystals of TTF-TCNQ Type for Different Values of Carrier Concentration

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Abstract

The Peierls structural transition is studied in quasi-one-dimensional (Q1D) organic crystals of the tetrathiofulvalene-tetracyanoquinodimethane (TTF-TCNQ) type in a more complete 2D physical model. Unlike the previous investigations, two electron-phonon interactions are considered: one is of the deformation potential type and the other is similar to that of polaron. The method of temperature Green functions is applied and the analytic expression for the polarization operator is obtained in the random phase approximation. The polarization operator as a function of temperature is calculated numerically for different values of the ratio d of the transfer energy in the direction transversal to conductive chains to the transfer energy along the conductive chains. The Peierls critical temperature Tp is determined for different values of the parameter d in two cases: 1) when the dimensionless Fermi momentum is kF = 0.59π/2, and 2) when the Fermi momentum is kF = 0.59π/2 ± δ, where δ represents the variation of the Fermi momentum, determined by the increase or by the decrease of carrier concentration. It is found that in the first case the Tp strongly decreases with the increase of the parameter d and for a certain value of the parameter d the Peierls transition does not take place on the whole. In the second case, the Tp with the increase of carrier concentration n also decreases and for some value of n the transition disappears too. But with the decrease of carrier concentration the Tp strongly increases. In both these cases the physical interpretations of such behavior of the Peierls transition are presented and discussed.