MODELING OF THE STRUCTURAL TRANSITION IN THE NANOSTRUCTURED TETRATHIOTETRACENE-IODIDE CRYSTAL

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The Peierls structural transition in quasi-one-dimensional (Q1D) organic crystals of tetrathiotetracene iodide (TTT_2I_3) is presented in the 1D and 2D physical model. For a more complete description of the crystal, two the main hole-phonon interactions are considered. The expression for the phonon polarization operator is obtained in the random phase approximation. Numerical calculations for the polarization operator as a function of temperature were performed for different values of parameter *d*, where *d* is the ratio of the transfer energy in the direction transversal to conductive chains to the transfer energy along the conductive chains. The behavior of Peierls transition is analyzed for different values of dimensionless Fermi momentum k_F. Different cases are studied: when $k_F = \pi/4$ and when the carrier concentration varies and $k_F = \pi/4 \pm \delta$**,** where δ represents the variation of Fermi momentum k_F. In all analyzed cases, the Peierls critical temperature T_p is determined.