Poster PS-12

Peierls Structural Transition in Quasi-One-Dimensional Organic Crystals of TTT_2I_3

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The Peierls structural transition in quasi-one-dimensional (Q1D) organic crystals of tetrathiotetracene iodide ($TTT_2I_{3.1}$) is presented in the 3D physical model. A more complete physical model of the crystal is applied, which takes into account two the main hole-phonon interactions. The

first interaction is similar to that of deformation potential and is determined by the variation of the transfer energy of a carrier from one molecule to the nearest one, caused by acoustic lattice vibrations. The second interaction is of polaron type and is determined by the variation of the polarization energy of molecules surrounding the conduction electron caused by the same acoustic vibrations. The scattering on structural defects is also taken into account, and it is shown that this interaction is crucial for the explanation of the Peierls structural transition in these crystals. Analytical expression for the polarization operator was obtained in random phase approximation. The method of retarded temperature dependent Green function is applied. The numerical calculations for renormalized phonon spectrum, $\Omega(q_x)$, for different temperatures are presented, where q_x is the projection of the phonon wave vector along conductive chains in x direction: 1) when the interaction between transversal chains is neglected ($q_y = 0$, $q_z = 0$) and 2) when interactions between the adjacent chains are considered ($q_y \neq 0$, $q_z \neq 0$). In both cases, the Peierls critical temperature is determined. In [1] the same dependences for 2D physical model are presented. It is demonstrated that the hole-phonon interaction and the interaction with the structural defects diminish $\Omega(q_x)$ and reduce the sound velocity in a large temperature interval.

[1] Silvia Andronic, Anatolie Casian, Metal-insulator transition of Peierls type in quasi-one-dimensional crystals of TTT_2I_3. Advances in Materials Physics and Chemistry, 2017, vol. 7, nr. 5, p. 212-222. doi:10.4236/ampc.2017.75017