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Phonons near Peierls Structural Transition in Quasi-One-Dimensional Organic Crystals of TTF-TCNQ

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Abstract

The Peierls structural transition in quasi-one-dimensional organic crystals of TTF-TCNQ is investigated in the frame of a more complete physical model. The two most important electron-phonon interaction mechanisms are taken into account simultaneously. One is similar of that of deformation potential and the other is of polaron type. For simplicity, the 2D crystal model is considered. The renormalized phonon spectrum and the phonon polarization operator are calculated in the random phase approximation for different temperatures. The effects of interchain interaction on renormalized acoustic phonons and on the Peierls critical temperature are analyzed.

Keywords

Quasi-One-Dimensional Organic Crystals, TTF-TCNQ, Peierls Transition, Interchain Interaction, Renormalized Phonons

1. Introduction

Quasi-one-dimensional (Q1D) organic materials have received much interest during the last years due to more diverse and often unusual properties manifested by them [1]-[3]. Besides, their properties can be easily manipulated and controlled by molecular chemistry methods. It has been also mentioned that the highly conducting Q1D organic crystals may have very prospective thermoelectric applications [4] [5]. The charge transfer compound TTF-TCNQ (tetrathiafulvalene-tetracyanoquinodimethane) is the most investigated Q1D organic crystal with the high electrical conductivity [6]. Its structure consists of segregated chains or stacks of TTF and TCNQ molecules. The metallic properties are due to partial transfer of electrons from TTF to TCNQ molecules.

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