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Electron-phonon coupling in potassium-doped superconducting picene MICHELE CASULA, MATTEO CALANDRA, FRANCESCO MAURI, CNRS and Université P. et M. Curie — We explore the properties of electron-phonon couplings in K_3Picene, in the framework of density functional theory (DFT). By exploiting the maximally localized Wannier function formalism, we identify the contribution of the intra- and intermolecular phonon vibrations and the role of local and non-local electronic states in determining the electron-phonon coupling. Despite the molecular nature of the crystal, we find that the purely molecular contributions account for only 20% of the total electron-phonon interaction λ. In particular, the Holstein-like contribution to λ are four times smaller than those computed for an isolated neutral molecule, as they are strongly screened by the metallic bands of the doped crystal. The major contribution (80%) to λ in K_3Picene comes from non-local couplings due to phonon modulated hoppings. We show that the crystal geometry together with the molecular picene structure leads to a strong 1D spatial anisotropy of the non-local couplings. Finally, we propose a lattice model of the electron-phonon couplings in K3Picene that gives 90% of the λ obtained in first principles calculations [1].

[1] M. Casula, M. Calandra and F. Mauri, PRL 107, 137006 (2011), PRB 86, 075445 (2012)

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