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The interaction of charge carriers with lattice phonons in oligoacene crystals VEACESLAV COROPCEANU, YUAN LI, YUANPING YI, ROBERT BROWN, JEAN-LUC BREDAS, Center for Organic Photonics and Electronics and School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA 30332-0400, USA — We use density functional theory calculations to investigate the non-local electron-phonon interactions between charge carriers and lattice phonons (i.e., the modulation of transfer integrals by vibrations) in oligoacene crystals as a function of molecular size from naphthalene through pentacene. The results point to a significant coupling to both translational and librational intermolecular phonon modes as well as to intra-molecular vibrational modes. The impact of the interplay among these mechanisms on charge transport is investigated by treating the lattice dynamics classically. The impact of quadratic electron-phonon interaction on charge transport is studied as well.

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