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Computational Study of Electron-Phonon Coupling in Crystalline Organic Semiconductors[1] NENAD VUKMIROVIC, Scientific Computing Laboratory, Institute of Physics Belgrade, University of Belgrade, Belgrade, Serbia, CHRISTOPH BRUDER, VLADIMIR M. STOJANOVIC, Department of Physics, University of Basel, Basel, Switzerland — Despite wide interest in organic molecular crystals and the recognition that electron-phonon (e-ph) coupling strength crucially determines the nature of charge carriers in these materials, ab-initio studies of e-ph coupling elements in these materials are still lacking. In this work [1], we calculated the e-ph coupling elements throughout the whole Brillouin zone in crystalline naphthalene using density functional perturbation theory within the generalized gradient approximation. Fourier-Wannier interpolation scheme [2] was then used to obtain the e-ph coupling constants on a fine k-point grid necessary for accurate evaluation of physical properties. Using the obtained e-ph coupling elements, we evaluated the quasiparticle residues for electrons and holes, obtaining the values of 0.74 and 0.78, respectively. These values suggest that e-ph coupling strength is insufficient for formation of small polarons in crystalline naphthalene and other oligoacene semiconductors. [1] N. Vukmirovic, C. Bruder, and V. M. Stojanovic, Phys. Rev. Lett. 109, 126407 (2012). [2] F. Giustino, M. L. Cohen, and S. G. Louie, Phys. Rev. B 76, 165108 (2007).

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