Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Electron-phonon coupling in naphthalene crystal ROEL SÁNCHEZ-CARRERA, PAVEL PARAMONOV, Department of Physics, University of Akron, Akron, Ohio 44325-4001, VEACESLAV COROPCEANU, JEAN-LUC BRÉDAS, School of Chemistry and Biochemistry and Center for Organic Photonics and Electronics, Georgia Institute of Technology, Atlanta, Georgia 30332-0400 — We investigate the electron interactions with optical phonons in crystalline naphthalene. The lattice phonon modes were computed at both DFT and empirical force field levels. The electron-phonon couplings were evaluated by means of numerical differentiation; in this approach, the crystal geometry is distorted along normal modes and transfer integrals for several selected molecular pairs are then computed at each distorted geometry. We find that the DFT and force field results for phonon frequencies and electron-phonon couplings compare very well. Interestingly, several phonon modes are calculated to display significant quadratic electron-phonon coupling. In addition, we have also performed electronic band-structure calculations and derived the effective masses for both electrons and holes.

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Date submitted: 26 Nov 2007 Electronic form version 1.4