Electron-Phonon coupling in naphtalene crystals

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We study the effect of electron-phonon interactions in naphthalene crystals, namely, the temperature-dependent renormalization of the band gap as well as the electron and hole mobilities. We take advantage of newly implemented interpolation schemes in Abinit for the phonon coupling potential, as well as an energy panelling technique for the real part of the self-energy. We show that special care has to be taken when converging the q-points grids, as both the coarse and the fine grids can have a dramatic impact on the mobilities. Moreover, we employ a self-consistent scheme for the electron-phonon coupling self-energy and the spectral function. It allows us to compare the accuracy of the on-the-mass-shell and the off-shell calculations.