Electron-phonon coupling in crystalline Pentacene films

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For decades theorists have been working to explain the surprisingly high carrier mobilities and temperature dependence of organic semiconductors (OSCs). Pioneering work toward understanding the carrier transport mechanism in OSCs was done by Holstein [1] in the 1950s. Holstein studied the influence of electron-phonon (e-p) interactions on mobilities for a model crystal and introduced the concept of a small polaron describing the incoherent contribution to carrier mobility. It was not until very recently that unified theories were developed considering both coherent and incoherent contributions to carrier mobility [2, 3]. In these unified theories low energy phonons and librations are able to both localize pure coherent states as well as assist the motion of less coherent ones. Although theories stress the importance of the e-p coupling in the transport properties of OSCs, surprisingly little work has been performed by experimentalists.

The present work reports temperature dependent photoemission data of the prototypical OSC Pentacene (Pn), and extracts the e-p interactions in a fashion similar to studies of various metals and semiconductors [4-7]. The electron-phonon (e-p) interaction in crystalline Pn films grown on Bi(001) was investigated using photoemission spectroscopy. The photoemission spectra reveal thermal broadening from which we determine an e-p mass enhancement factor of $\lambda = 0.36 \pm 0.05$ and an effective Einstein energy of $\omega_E = 11 \pm 4$ meV. Based on the experimental data for $\lambda$ we extract an effective Peierls coupling value of $g_{\text{eff}} = 0.55$. The e-p coupling narrows the HOMO bandwidth by 15% between 75 K and 300 K.

References