

Intermediate polaronic charge transport in organic crystals from a many-body first-principles approach (Supplementary Information)

Benjamin K. Chang,¹ Jin-Jian Zhou,¹ Nien-En Lee,¹ and Marco Bernardi^{1,*}

¹*Department of Applied Physics and Materials Science,
California Institute of Technology, Pasadena, California 91125, USA*

ELECTRON-PHONON COUPLING STRENGTH

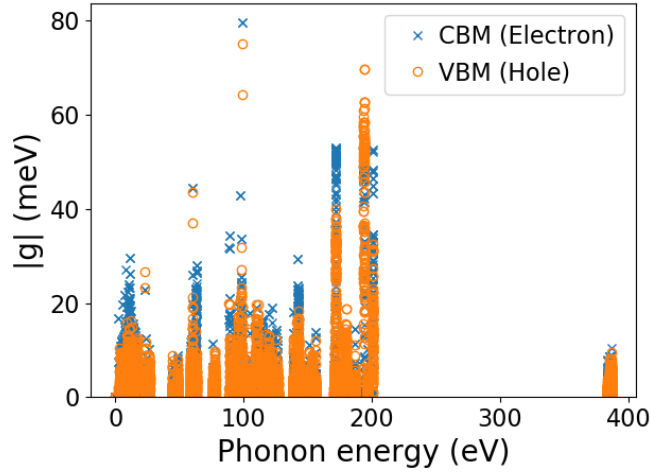


FIG. 1. Comparison of the e-ph coupling strength, quantified by the absolute values of the e-ph matrix elements, $|g|$, for the valence band maximum (VBM) hole state and the conduction band minimum (CBM) electron state. The electrons exhibit an overall stronger coupling with phonons with energies between 0–200 meV, which, combined with the greater electron effective mass (see Figure 1 in the main text), leads to a polaronic transport regime and the failure of the bandlike picture for electron carriers.

* bmarco@caltech.edu