

Conduction band structure of organic semiconductors and partially-dressed polaron formation

Haruki Sato¹, Syed A. Abd. Rahman¹, Yota Yamada¹, Hiroyuki Ishii², Hiroyuki Yoshida^{1,3*}

¹ *Graduate School of Engineering, Chiba University, Japan*

² *Faculty of Pure and Applied Sciences, University of Tsukuba, Japan*

³ *Molecular Chirality Research Center, Chiba University, Japan*

*E-mail: hyoshida@chiba-u.jp

The energy band structure (the energy-momentum dispersion relation) provides crucial information on charge transport in organic semiconductors, such as transfer integrals and electron-phonon coupling. Whereas the experimental observation of the valence band (HOMO) structure has been reported since the 1990s, the conduction band (LUMO) has yet to be experimentally observed.

Recently, we have developed angle-resolved low-energy inverse photoelectron spectroscopy (ARLEIPS) [1]. We apply ARLEIPS to pentacene, a prototypical high-mobility organic semiconductor, to successfully observe the conduction band structure of organic semiconductors for the first time [2]. To address the observed bandwidths, we propose an improved (partially-dressed) polaron model that accounts for the electron-intramolecular vibrational interaction with frequency-dependent coupling constants.

References

- [1] Kashimoto, Y.; Ideta, S.; Sato, H.; Orio, H.; Kawamura, K.; Yoshida, H. *Rev. Sci. Instrum.*, **94**, 063903 (2023). Selected as Editor's Pick
- [2] Sato, H.; Abd. Rahman, S. A.; Yamada, Y.; Ishii, H.; Yoshida, H. *Nature Mat.* **21**, 910 (2022).