Exploring function and property of organic materials by photoelectron spectroscopy

IMS [1], SOKENDAI [2], Chiba Univ [3], Satoshi Kera[1,2,3]

E-mail: kera@ims.ac.jp

Deep insight into important characters of functions and electronic properties for condensed molecular solids and their interfaces related has been achieved by using ultraviolet photoelectron spectroscopy (UPS). The energy position, intensity and width of the highest occupied molecular orbital (HOMO) band in UPS spectra of organic materials have in principle a variety of information that is directly related to energetics and carrier transport properties in organic-based devices. Especially the bandwidth and its profile reflect carrier dynamics through dynamic initial- and final-state effects in photoemission. Thus careful analyses of the spectra measured for well-defined organic films (single crystals) can offer crucial information that has not been obtained from usual UPS studies. We believe that understanding the impacts of strong electron-phonon coupling as well as weak electronic coupling (intermolecular interaction) on the electronic state is required to discuss peculiar properties eg., giant Seebeck effects, dopant tuning/control and charge transport mechanism in functional molecular materials. However, the experimental study of the fine features in the HOMO state by advanced UPS has not been progressed till recently due to difficulty in the sample preparation, damages upon irradiation and so on. We have discussed i) band position; role of molecular dipole and quadrapole on the energy levels [1,2], ii) band intensity; quantitative measurements of the density-of states to realize the energy-level alignment [3] and molecular orbital distribution [4], and iii) band shape; evolution of the charge localization from the state splitting to energy-band dispersion [5] and impacts of molecular vibration and lattice phonons on the charge transport [6,7]. The findings would help to recognize an electron in a molecular assemble, hence to design a new class of materials and hold complicating charge transport mechanism in fundamental.

[1] S. Kera, Y. Yabuuchi, H. Yamane, H. Setoyama, K.K. Okudaira, A. Kahn, N. Ueno, *Phys. Rev. B* **70**, 085304 (2004).
[2] C. Gaul, M. Schwarze, S. Schellhammer, F. Bussolotti, S. Kera, Z. Bao, G. Cuniberti, K. Leo, F. Ortmann, *Nat. Mater.* **17**, 439 (2018).
[3] J-P. Yang, F. Bussolotti, S. Kera, N. Ueno, *J. Phys. D: Appl. Phys.* **50**, 42300 (2017).
[4] Y. Liu, D. Ikeda, S. Nagamatsu, T. Nishi, N. Ueno, S. Kera, *J. Electron Spect. Relat. Phenom.* **195**, 287 (2014).
[5] Y. Kashimoto, K. Yonezawa, M. Meissner, M. Gruenewald, T. Ueba, S. Kera, R. Forker, T. Fritz, and H. Yoshida, *J. Phys. Chem. C* **122**, 12090 (2018).
[6] S. Kera and N. Ueno, *J. Electron Spectrosc. Relat. Phenom.* **204**, 2 (2015).
[7] F. Bussolotti, J. Yang, T. Yamaguchi, Y. Nakayama, M. Matsunami, H. Ishii, N. Ueno, S. Kera, *Nat. Comm.* **8**, 173 (2017).