Tracking charge transport of organic semiconductor material by electronic structure measurement

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Understanding the impacts of strong electron-phonon coupling as well as weak electronic interaction on the electronic state is required to discuss the rich of functionality in organic molecular materials. Angle-resolved ultraviolet photoelectron spectroscopy (ARUPS) is known to be a powerful technique to study the electronic states. The valence-band features can offer a wide variety of key information, that is essential to comprehend charge-hopping transport and small-polaron related transport in the ordered monolayer film [1,2] as well as to coherent band transport in the molecular single crystal [3]. However, the experimental study of fine features in the frontier orbital state has not been progressed till recently due to difficulty in the high quality sample preparation, damages upon irradiation, and so on. We present recent findings regarding on the precise measurements of electronic states for rubrene molecule by using low-energy excited, high-resolution ARUPS. The photoelectron angular distribution, that is relation between photoelectron kinetic energy or photoelectron intensity and momentum (photoemission angle), gives fruitful information of orbital distribution, electron effective mass, and transfer integral. For the well-ordered monolayer crystal films, strong fine features of the satellite bands based on Franck-Condon factor are detected due to a weak electronic interaction by anti-π-stacking orientation. The charge reorganization energy is evaluated by analyzing the intensity progression, where the values are depending on the molecular orientation/packing because of a rich flexibility of the molecular backbone [4,5]. For the single crystal bulk sample, a clear energy-band dispersion of a quasiparticle state is observed in the ARUPS, where the effective mass is renormalized by intermolecular and intramolecular electron-phonon couplings [6,7]. By considering the effects of local and non-local vibration on the electronic structure, a perspective of designing the high-performance organic semiconductor devices would be described.

References

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