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Photoemission study on the charge transport mechanism in pentacene thin film¹

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Organic molecules are attracting much interest to use for a variety of electronic applications. Pentacene (Pn), which is one of such molecules, has a high application potential due to its high hole mobility. The hole mobility of Pn is almost comparable to that of amorphous silicon. At low temperature, the hole transport in Pn crystal has been reported to have a band-like nature, and the band-like charge transport is expected to play a major part at room temperature as well. One of the origins of the band-like transport is the adequate overlap of the pi-orbitals of adjacent molecules, which produces orbital-derived electronic bands. It is therefore essential to have a proper understanding on the electronic band structures in order to fully comprehend the charge transport mechanism of a Pn crystal. By using angle-resolved photoelectron spectroscopy (ARPES), we have measured the dispersions of the highest occupied molecular orbital (HOMO)-derived bands of single crystal Pn monolayer films grown on substrates. Two HOMO-derived, whose band dispersion widths are larger than the values predicted by theoretical calculations, were clearly observed in the ARPES spectra. Our result indicates that the overlap of the pi-orbitals of adjacent Pn molecules is larger than what was expected from theoretical calculations, and the observed dispersions suggest that the higher binding energy HOMO-derived band mainly contributes to the band-like charge transport mechanism of a Pn crystal. By analyzing the dispersions within a simple tight-binding approximation, the obtained results lead to a hole mobility of $mu_h > 34.1 \text{ cm}^2/\text{Vs}$ at 140 K.

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