

## Molecular orientation of pentacene derivative

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### Introduction

Organic electrically conducting  $\pi$ -stacked small molecules are widely regarded as promising materials for future application of low-cost and flexible nanoelectronics. Pentacene is one of the most promising organic semiconductors because of its excellent device performance. Direct measurements of electronic structures of unoccupied states of organic semiconductors lead to better understanding of mechanism of electron conduction. For probing unoccupied partial density of states (DOS), X-ray absorption spectroscopy (XAS) is commonly used, where selective excitation of the 1s core electron to the unoccupied conduction band is possible.

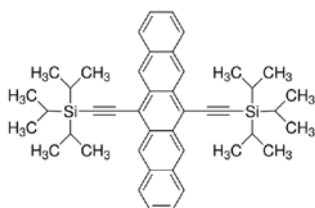
Pentacene shows an edge-to-face herringbone arrangement in crystal. Nevertheless, a soluble pentacene derivative, 6,13-bis(triisopropylsilyl)ethynyl pentacene (TIPS-pentacene) with a pentacene backbone and two bulky side groups, shows a face-to-face  $\pi$ - $\pi$  stacking arrangement [1]. The molecular orientation of TIPS-pentacene has been investigated by angle dependent XAS measurements.

### Experimental

Experiments were performed at beamline BL-27A with energy resolution of 0.9 eV. The XAS spectra were measured using monitoring sample drain current near the Si K-edge (1835–1880 eV). Such energies were chosen to excite the Si 1s core electron to unoccupied orbitals of TIPS-pentacene. The as-received powdered sample was pressed on conductive carbon tapes. Angle dependent XAS data of TIPS-pentacene polycrystalline powder were obtained by changing the angle between the incoming X-ray beam and the sample surface.

### Results and discussion

Figure 1 shows the Si K-edge XAS spectra of TIPS-pentacene polycrystalline powder at different incident angles of X-ray incidence  $\theta$ , between the direction of propagation of incident synchrotron light X-ray and the surface plane. The XAS spectral intensity of TIPS-pentacene changes at peaks 1 and 3, which indicate



TIPS-pentacene

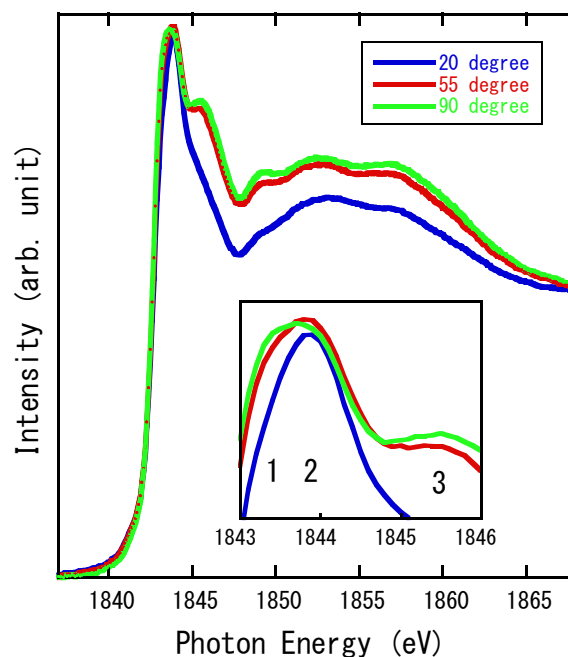


Fig.1 XAS spectra of TIPS-pentacene polycrystalline powder as a function of angle of X-ray incidence near the Si K-edge.

that crystalline domains of TIPS-pentacene are relatively aligned on surface plane. Peaks 1 and 3 are enhanced at the normal incidence of the X-ray, while peak 2 shows no polarization dependence. Peaks 1 and 3, and higher energy peaks (1850–1860 eV) can be mainly assigned to excitations with parallel transition dipole moment to the pentacene backbone (transition along long axis). On the other hand, peak 2 can be mainly assigned to an excitation with perpendicular transition dipole moment to the pentacene backbone (transition along short axis). These assignments have been made with use of self-consistent local-density theory with the discrete variational (DV- $X\alpha$ ) method. As a result of the angle dependent XAS data, TIPS-pentacene is found to be aligned with its long molecular axis oriented parallel to the surface.

### References

- [1] J.E. Anthony, *Chem. Rev.* **106**, 5028 (2006).

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