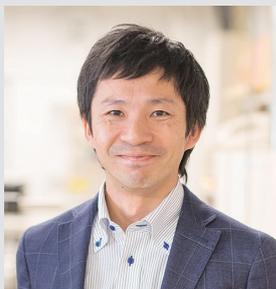


Electronic Property of Functional Low-Dimensional Material Systems

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Functional low-dimensional material systems (LMS) such as oriented molecular assembles on the surface have recently attracted considerable attention both for fundamental research and device applications because of peculiar properties not found in bulk materials or small molecules. However, the mechanisms and the origin of various device characteristics are still under debate. Scientific discussions have been redundant because of long-standing beliefs that the electronic structure would be conserved as in an isolated molecule even for solid phases due to the weak van der Waals interaction. To reveal characteristics of the LMS, it is essential to investigate precisely the electronic structure at various interfaces, including organic–organic and organic–inorganic (metal/semiconductor) contacts. Recently we realized that the weak electronic interaction manifests itself as small intensity modulations of fine structures in photoelectron spectra, depending on the adsorption and aggregation conditions on the surface. Thanks to recent instrumentation improvements, we can assess hidden fine features in the electronic states, e.g. electron–phonon coupling, quasi-particle states, very small densities of gap states, narrow band dispersion, and dynamic electronic polarization. To elucidate what really impacts on the electronic states of the LMS as well as at the interface upon weak interaction, an evaluation of the wave-function spread of the electronic states

is very important because the interface states are described as a delocalized molecular orbital state depending on the strength of weak electronic coupling (hybridization). Observing modifications of electron wave functions upon weak electronic coupling as well as strong electron–phonon coupling is a central issue on our agenda (Figure 1).

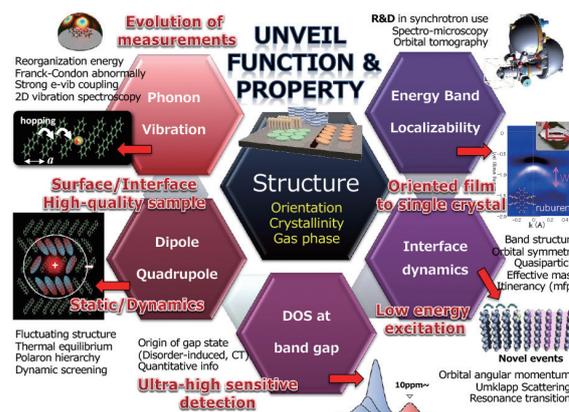


Figure 1. Overview of our agenda. A rich assortment of surface and interface structures of LMS to provide complicated spectral features of ultraviolet photoelectron spectroscopy.

Selected Publications

- Y. Nakayama, S. Kera and N. Ueno, *J. Mater. Chem. C* **8**, 9090–9132 (2020). [review]
- S. Kera, T. Hosokai and S. Duhm, *J. Phys. Soc. Jpn.* **87**, 061008 (7 pages) (2018). [review]
- J.-P. Yang, F. Bussolotti, S. Kera and N. Ueno, *J. Phys. D: Appl. Phys.* **50**, 423002 (45 pages) (2017). [review]
- S. Kera and N. Ueno, *J. Electron Spectrosc. Relat. Phenom.* **204**, 2–11 (2015). [review]

1. Enantiospecific Mirror-Imaged Growth in Overlayers of Enantiopure Helicene on Au(111) without Commensurability¹⁾

Two-dimensional crystallization of chiral molecules on achiral crystal surfaces typically exhibits mirror-imaged growth, defined by the substrate's mirror plane and the lattices of each enantiomer. While various commensurate molecular overlayers have shown such growth, the possibility of achieving substrate-defined enantiospecific structures in non-commensurate chiral molecular overlayers remains elusive. Here, enantiopure thiadiazole-[9]helicene on Au(111) is shown to form overlayers without commensurability, exhibiting substrate-defined mirror-imaged growth (Figure 2). This study experimentally demonstrates that the rotational orientation locking without two-dimensional interface potential minima can support mirror-imaged growth, suggesting that it can serve as benchmark for enantiospecific growth in a broader range of chiral molecular systems. The well-defined chiral molecular system will be useful for studying the mechanisms of chirality-induced spin selectivity at the interface in the near future.

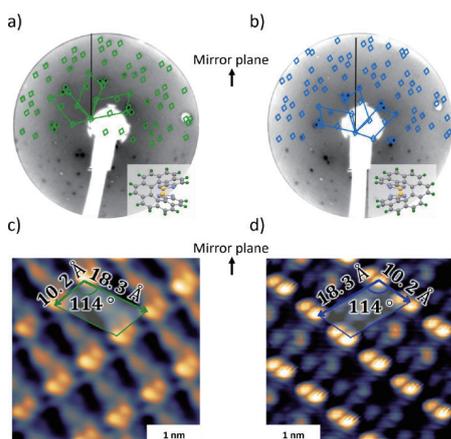


Figure 2. (a) and (b) are the distortion-corrected LEED images for (M)-TD[9]H and (P)-TD[9]H molecular layers on Au(111), observed at beam energies of 39.5 eV and 41.5 eV, respectively. (c) and (d) are STM images of (M)-TD[9]H and (P)-TD[9]H layers, respectively. The figure is after ref 1).

2. Fingerprinting Weak Electronic Interaction at a van der Waals Interface: Fano Signatures in Pentacene Monolayer on Graphite²⁾

The influence of van der Waals (vdW) interactions on the electronic structure at the interface between a pentacene monolayer and a graphite surface was investigated by using high-resolution angle-resolved photoelectron spectroscopy (ARPES) with synchrotron light sources. Upon cooling below

130 K, the pentacene molecules form a densely packed monolayer characterized by newly developed dispersive bands. These bands, observed using low-energy ARPES with photon energy varying from 7.2 to 8.5 eV, exhibit constant final state characteristics that overlap with nondispersive molecular orbital states (Figure 3). The results in variations for the photoemission intensity, both enhancement and suppressions the photoemission intensity, indicative of Fano resonance. Such resonance arises from the interaction between a discrete molecular state and a continuum state. The Fano profile analysis of spectral fine features reveals the wave-function connection by the broader spread in unoccupied states at the physisorbed interface. This discovery underscores the significant role of weak electronic coupling in shaping wave function connectivity, highlighted by the broader spread of unoccupied states. This spread serve as a spectral fingerprint for proving weak interactions at the vdW interface. The asymmetric parameter will provide quantifiable metrics for characterizing weak interactions, with further theoretical developments anticipated.

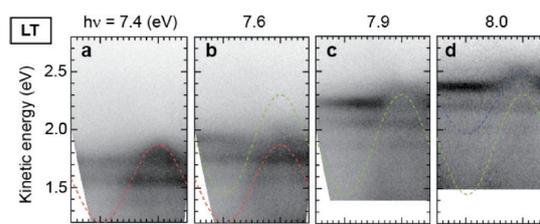


Figure 3. Photon energy dependence of the E - k map of pentacene on graphite (HOPG) recorded at LT (50 K for 8.0 eV and 14 K for 7.4, 7.6, and 7.9 eV) along with the fitting curves (POS: blue and red, NEG: green). The figure is after ref 2).

3. Other Activities in UVSOR

We have conducted beamline R&D and user supports in collaboration with other universities. Experiments using photoelectron momentum microscope are developing at BL6U.³⁾ The perspectives required for future light-source facility have been discussed with communities.

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- 2) Y. Hasegawa, T. Yamaguchi, M. Meissner, T. Ueba, F. Bussoloti, S. Ideta, K. Tanaka, S. Yanagisawa and S. Kera, *Phys. Rev. B* **112**, 085301 (2025).
- 3) K. Hagiwara, E. Nakamura, S. Makita, S. Suga, S. Tanaka, S. Kera and F. Matsui, *J. Synchrotron Radiat.* **31**, 540 (2024).

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