

Visiting Professors



Visiting Professor

MATSUSHITA, Tomohiro (*from Nara Institute of Science and Technology*)

Development of Analysis Methods for Photoelectron Momentum Microscope

Following last year, we have continued the development of data analysis tools for the photoelectron momentum microscope introduced at UVSOR. This instrument is a highly powerful tool for observing the electronic structure of samples, including spin, by means of photoelectron spectroscopy. Using the first-principles calculation code OpenMX, we have enabled the calculation of photoelectron transition probabilities, so that the observed photoelectron intensities from the valence band can be analyzed. We have begun comparing the experimental results of twisted graphene obtained using the momentum microscope with theoretical calculations. In addition, we applied principal component analysis to the 1T-TaS₂ data obtained with this instrument, attempting to visualize the behavior of the phase transition. In this way, we are developing a framework that integrates first-principles calculations with information-theoretical approaches.



Visiting Associate Professor

SHIBUTA, Masahiro (*from Osaka Metropolitan University*)

Vibration-Resolved Unoccupied Molecular Orbitals by Two-Photon Photoemission Spectroscopy

Carrier-vibration couplings in organic thin films are important to understand the carrier mobilities in organic devices. So far, hole-vibration couplings have been studied, resolving fine structures of occupied orbitals using photoelectron spectroscopy. However, it was difficult to analyze electron–vibration couplings because we must analyze the unoccupied orbitals. Two-photon photoemission (2PPE) spectroscopy is a powerful method to observe unoccupied states with high resolution (20 meV), where a first photon injects an electron from a substrate into an adsorbed molecule, and the excited electron is extracted by a second photon. In fact, we have successfully resolved fine structures in the lowest unoccupied molecular orbital (LUMO)-derived peaks for small polyaromatic molecular films (*e.g.*, naphthalene, anthracene, phenanthrene) due to electron–vibration couplings. These results are opening the door to understand the electron mobility in the organic films. Furthermore, 2PPE can track the time-dependent behavior of the fine structures, which will unveil the energy modification and/or molecular motion of the excited state in the ultrafast regime.