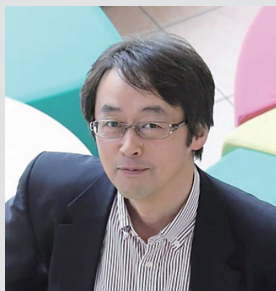


Exploring Novel Physical Properties by Multi-Dimensional Spectroscopy

**Division of Advanced Molecular Science
(Department of Materials Molecular Science, Electronic Structure)**



KIMURA, Shin-ichi
Professor
(Cross Appointment)
[kimura@ims.ac.jp]

Education

1988 B.S. Tohoku University
1990 M.S. Tohoku University
1991 Ph.D. Tohoku University

Professional Employment

1991 JSPS Postdoctoral Fellow, Tohoku University
1993 Research Associate, Kobe University
1993 Research Associate, Institute for Molecular Science
1998 Associate Professor, Kobe University
2002 Associate Professor, Institute for Molecular Science
2013 Professor, Osaka University
2020 Professor (Cross Appointment), Institute for Molecular Science

Awards

2001 Young Incentive Award, Japanese Society for Synchrotron Radiation Research
2008 The Commendation for Science and Technology by MEXT, Japan Science and Technology Prize (Research Field)
2008 Morita Memorial Prize

Member
Secretary
ISHIKAWA, Azusa

Keywords Condensed Matter, Optical and Photoelectrical Properties, Synchrotron Radiation

Physical and chemical properties of solids, such as conductivity, magnetism, superconductivity and chemical reactions originate from microscopic electronic structure, lattice/molecular vibrations, and molecular movements based on quantum mechanics in materials and their interactions. By revealing the microscopic states, we can learn about the origin of physical and chemical properties and hidden functionalities. Also, the microscopic information is helpful for the creation of novel functional properties. To visualize hidden microscopic information, we develop novel spectroscopic techniques using synchrotron radiation, high brilliant electron beams, and other so-called quantum beams. We are now developing a new electron spectroscopy technique, namely Spin-Resolved resonant Electron-Energy-Loss Spectroscopy (SR-rEELS), with bulk-sensitive primary energies of 0.3–1.5 keV, as shown in Figure 1, in order to detect spin-selective element-specific bulk plasmons. Based on the obtained information of electronic structures, we aim to develop novel physical properties of new materials.

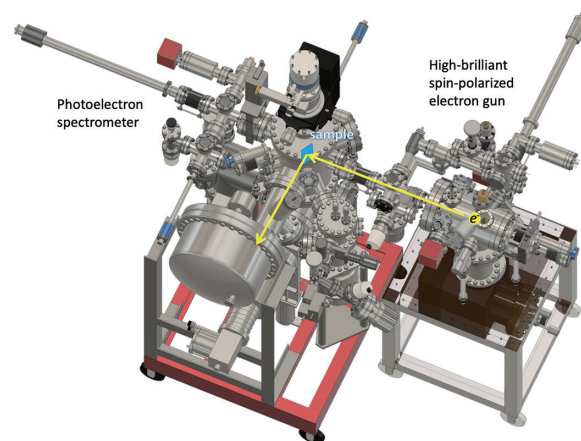


Figure 1. Spin-Resolved resonant Electron-Energy-Loss Spectroscopy (SR-rEELS) apparatus developed by our group. The apparatus consists of a high-brilliant spin-polarized electron gun and a photoelectron spectrometer.

Selected Publications

- Y. Ohtsubo, Y. Yamashita, K. Hagiwara, S. Ideta, K. Tanaka, R. Yukawa, K. Horiba, H. Kumigashira, K. Miyamoto, T. Okuda, W. Hirano, F. Iga and S. Kimura, “Non-Trivial Surface States of Samarium Hexaboride at the (111) Surface,” *Nat. Commun.* **10**, 2298 (7 pages) (2019).
- K. Hagiwara, Y. Ohtsubo, M. Matsunami, S. Ideta, K. Tanaka, H. Miyazaki, J. E. Rault, P. Le Fèvre, F. Bertran, A. Taleb-Ibrahimi, R. Yukawa, M. Kobayashi, K. Horiba, H. Kumigashira, K. Sumida, T. Okuda, F. Iga and S. Kimura, “Surface Kondo Effect and Non-Trivial Metallic State of the Kondo Insulator YbB_{12} ,” *Nat. Commun.* **7**, 12690 (7 pages) (2016).
- S. Kimura and H. Okamura, “Infrared and Terahertz Spectroscopy of Strongly Correlated Electron Systems under Extreme Conditions,” *J. Phys. Soc. Jpn.* **82**, 021004 (28 pages) (2013). [review]
- S. Kimura, T. Iizuka, H. Miyazaki, A. Irizawa, Y. Muro and T. Takabatake, “Electronic-Structure-Driven Magnetic Ordering in a Kondo Semiconductor $\text{CeOs}_2\text{Al}_{10}$,” *Phys. Rev. Lett.* **106**, 056404 (4 pages) (2011).

1. Magneto-Optics of the Weyl Semimetal TaAs in the THz and IR Regions¹⁾

The magnetic-field dependence of optical conductivity [$\sigma(\omega)$] spectra of the ideal type-I Weyl semimetal TaAs has been investigated at the temperature of 10 K in the terahertz (THz) and infrared (IR) regions. The obtained $\sigma(\omega)$ spectrum in the THz region of $\hbar\omega \leq 15$ meV is strongly affected by the applied magnetic field (B): The Drude spectral weight is rapidly suppressed, and an energy gap originating from the optical transition in the lowest Landau levels appears with a gap size that increases in proportion to \sqrt{B} , which suggests linear band dispersions. The obtained THz $\sigma(\omega)$ spectra could be scaled not only in the energy scale by \sqrt{B} but also in the intensity by $1/\sqrt{B}$ as shown in Figure 2, which has been predicted theoretically. In the IR region for $\hbar\omega \geq 17$ meV, on the other hand, the observed $R(\omega)$ peaks originating from the optical transitions in higher Landau levels are proportional to linear- B suggesting parabolic bands. The different band dispersions suggests that the Dirac linear bands transition to the free-electron-like parabolic bands with increasing energy.

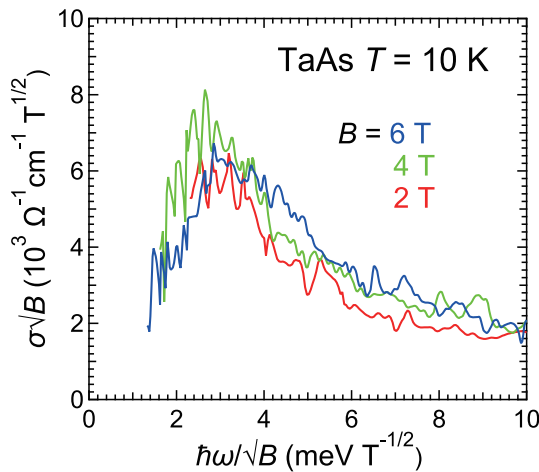


Figure 2. Magnetic-field dependence of optical conductivity [$\sigma(\omega, B)$] spectrum of TaAs in the THz region at the temperature of 10 K. The horizontal and vertical axes are normalized by B and $1/\sqrt{B}$, respectively.

2. One-Dimensionality of the Spin-Polarized Surface Conduction and Valence Bands of Quasi-One-Dimensional Bi Chains on GaSb(110)-(2×1)²⁾

Surface electronic structure and its one-dimensionality above and below the Fermi level (E_F) are surveyed on the Bi/GaSb(110)-(2×1) surface hosting quasi-one-dimensional (Q1D) Bi chains, using conventional (one-photon) and two-photon angle-resolved photoelectron spectroscopy (ARPES) and theoretical calculations. ARPES results reveal that the Q1D electronic states are within the projected bulk band gap. Circular dichroism of two-photon ARPES and density-functional-theory calculation indicate clear spin and orbital polarization of the surface states consistent with the giant sizes of

Rashba-type spin-orbit interaction (SOI), derived from the strong contribution of heavy Bi atoms. The surface conduction band above E_F forms a nearly straight constant-energy contour (Figure 3a), suggesting its suitability for application in further studies of one-dimensional electronic systems with strong SOI. A tight-binding model calculation based on the obtained surface electronic structure successfully reproduces the surface band dispersions (Figures 3b, 3c) and predicts possible one- to two-dimensional crossover in the temperature range of 60–100 K.

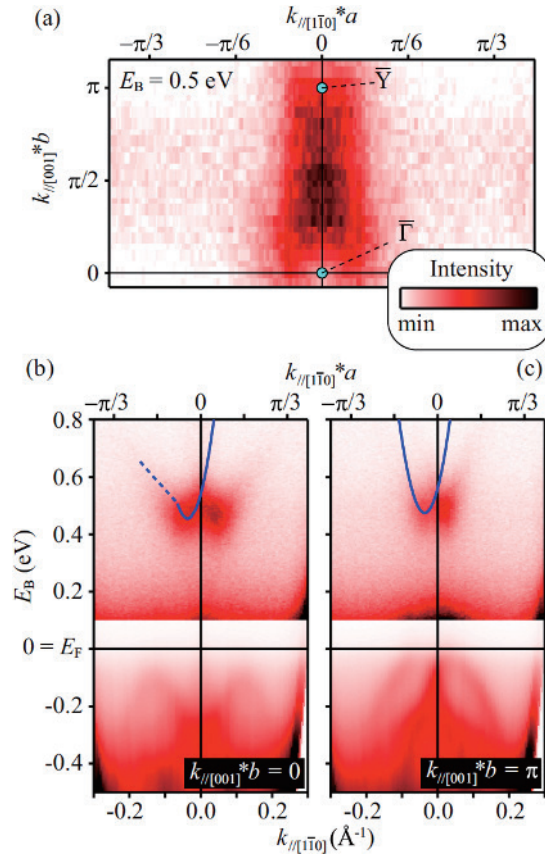


Figure 3. ARPES intensity plots of Bi/GaSb(110)-(2×1) at 25 K taken with two laser pulses. A delay time between the pump and probe pulses was set to 1 ps. The pump pulses ($\hbar\nu = 1.5$ eV) were linearly polarized photons, the electric field vector, which lies in the photon incident plane. The probe ones had the same incident plane as the circular polarization ($\hbar\nu = 6.0$ eV). (a) Constant energy contour at $E_B \sim 0.5$ eV. (b) ARPES intensity plot along $\bar{\Gamma}-\bar{X}$. The photoelectron signals in $E_B > 0.1$ eV are enhanced to make the surface conduction band dispersion visible. (c) Same as (b) but taken along $\bar{Y}-\bar{M}$. Solid and dashed curves in (b) and (c) guide the theoretical band dispersions.

References

- 1) S. Kimura, Y. Yokoyama, Y. Nakajima, H. Watanabe, J. Sichelschmidt, V. Süß, M. Schmidt and C. Felser, *JPS Conf. Proc.* **30**, 011017 (5 pages) (2020).
- 2) Y. Ohtsubo, N. Tokumasu, H. Watanabe, T. Nakamura, P. Le Fèvre, F. Bertran, M. Imamura, I. Yamamoto, J. Azuma, K. Takahashi and S. Kimura, *Phys. Rev. B* **101**, 235306 (8 pages) (2020).