

# Publications

## Division of Condensed Matter Science

### Takigawa group

We have been performing nuclear magnetic resonance experiments on various quantum spin systems and strongly correlated electron systems to explore novel quantum phases with exotic ordering and fluctuation phenomena. The major achievements in the year 2015 include: (1) Discovery of a magnetic field-induced phase transition in PrTi<sub>2</sub>Al<sub>20</sub>, a f-electron system with the Gamma-3 non-magnetic doublet crystal field ground state, by means of Al-NMR and magnetization measurements. (2) First observation of a magnetic order in the heavy electron system beta-YbAlB<sub>4</sub> under high pressure of 8 GPa.

1. \* NMR Observation of Ferro-Quadrupole Order in PrTi<sub>2</sub>Al<sub>20</sub>: T. Taniguchi, M. Yoshida, H. Takeda, M. Takigawa, M. Tsujimoto, A. Sakai, Y. Matsumoto and S. Nakatsuji, J. Phys. Soc. Jpn. **85** (2016) 113703(1-4).
2. Pressure-Tuned Exchange Coupling of a Quantum Spin Liquid in the Molecular Triangular Lattice  $\kappa$ -(ET)<sub>2</sub>Ag<sub>2</sub>(CN)<sub>3</sub>: Y. Shimizu, T. Hiramatsu, M. Maesato, A. Otsuka, H. Yamochi, A. Ono, M. Itoh, M. Yoshida, M. Takigawa, Y. Yoshida and G. Saito, Phys. Rev. Lett. **117** (2016) 107203(1-6).
3. \* Single crystal <sup>27</sup>Al-NMR study of the cubic  $\Gamma_3$  ground doublet system PrTi<sub>2</sub>Al<sub>20</sub>: T. Taniguchi, M. Yoshida, H. Takeda, M. Takigawa, M. Tsujimoto, A. Sakai, Y. Matsumoto and S. Nakatsuji, J. Phys.: Conf. Ser. **683** (2016) 012016(1-9).
4. \* Site-selective <sup>11</sup>B NMR studies on YbAlB<sub>4</sub>: S. Takano, M. S. Grbic, K. Kimura, M. Yoshida, M. Takigawa, E. C. T. O. Farrell, K. Kuga, S. Nakatsuji and H. Harima, J. Phys.: Conf. Ser. **683** (2016) 012008(1-6).
5. J(1)-J(2) square-lattice Heisenberg antiferromagnets with 4d(1) spins AMoOPO(4)Cl (A=K, Rb): H. Ishikawa, N. Nakamura, M. Yoshida, M. Takigawa, P. Babkevich, N. Qureshi, H. M. Rønnow, T. Yajima and Z. Hiroi, Phys. Rev. B **95** (2017) 064408.

### Sakakibara group

We study magnetism and superconductivity of materials having low characteristic temperatures. These include heavy-electron systems, quantum spin systems and frustrated spin systems. The followings are some selected achievements in the fiscal year 2016. (1) An experimental technique of low-temperature magnetization measurements under in-situ tuning of the sample orientation has been developed. A two-axis goniometer is introduced into our capacitively-detected Faraday magnetometer, making it possible to rotate the sample by  $|\theta| < 7$  deg. and  $|\phi| < 3$  deg. The apparatus has been applied to a metamagnetic heavy fermion compound CeRu<sub>2</sub>Si<sub>2</sub>, and found that the magnetization isotherms  $M(H)$  of this tetragonal compound can be completely scaled by  $H \cos \theta$ , where  $\theta$  is the angle between  $H$  and the  $c$  axis, confirming the Ising nature of this system. (2) The critical exponent  $\nu$  of the phase boundary of a field-induced incommensurate ordering state has been examined on the spin-1/2 ferromagnetic-leg ladder 3-Br-4-F-V [=3-(3-bromo-4-fluorophenyl)-1,5-diphenylverdazyl]. Using the temperature-window fitting technique, we obtained the critical exponents which agreed with the 3D Bose-Einstein condensation (BEC) universality class at both sides of the lower critical field and the saturation field. 3-Br-4-F-V thus becomes a new member of the quantum magnets which prove the universality of the 3D BEC exponent. (3) Quasiparticle excitations in the hexagonal heavy-fermion superconductor UPd<sub>2</sub>Al<sub>3</sub> have been studied by means of heat capacity ( $C$ ) measurements under rotating magnetic fields. At low temperatures, the polar angle ( $\theta$ ) dependence of  $C$  exhibits a maximum along  $H \parallel [0001]$  with a two-fold symmetric oscillation below 0.5 T, and an unusual shoulder/hump anomaly has been found around 30-60 deg. from the  $c$  axis in  $C(\theta)$  at intermediate fields ( $1 < H < 2$  T). This feature in  $C(\theta)$  entirely comes from nodal quasiparticle excitations, and has been successfully explained by theoretical calculations assuming a gap function with a horizontal line node.

1. Evidence for chiral  $d$ -wave superconductivity in URu<sub>2</sub>Si<sub>2</sub> from the field-angle variation of its specific heat: S. Kittaka, Y. Shimizu, T. Sakakibara, Y. Haga, E. Yamamoto, Y. Onuki, Y. Tsutsumi, T. Nomoto, H. Ikeda and K. Machida, J. Phys. Soc. Jpn. **85** (2016) 033704 (2016).
2. †\* Superconductivity and Non-Fermi-Liquid Behavior in the Heavy-Fermion Compound CeCo<sub>1-x</sub>Ni<sub>x</sub>In<sub>5</sub>: R. Otaka, M. Yokoyama, H. Mashiko, T. Hasegawa, Y. Shimizu, Y. Ikeda, K. Tenya, S. Nakamura, D. Ueta, H. Yoshizawa and T. Sakakibara, J. Phys. Soc. Jpn. **85** (2016) 094713.

\* Joint research among groups within ISSP.

3. Field-induced phase transitions and magnetoferroelectricity in the perfect triangular lattice antiferromagnet  $\text{RbFe}(\text{MoO}_4)_2$  in a vertical magnetic field: H. Mitamura, R. Watanuki, N. Onozaki, Y. Amou, Y. Kono, S. Kittaka, Y. Shimura, I. Yamamoto, K. Suzuki and T. Sakakibara, *J. Magn. Magn. Mater.* **400** (2016) 70-72.
4. First-order superconducting transition of  $\text{Sr}_2\text{RuO}_4$  investigated by magnetization and magnetic torque: S. Kittaka, A. Kasahara, T. Sakakibara, D. Shibata, S. Yonezawa, Y. Maeno, K. Tenya and K. Machida, *J. Magn. Magn. Mater.* **400** (2016) 81-83.
5. Heat capacity measurements on  $\text{UBe}_{13}$  in rotated magnetic fields: anisotropic response in the normal state and the absence of nodal quasiparticles: Y. Shimizu, S. Kittaka, T. Sakakibara, Y. Haga, E. Yamamoto, H. Amitsuka, Y. Tsutsumi and K. Machida, *J. Magn. Magn. Mater.* **400** (2016) 52-55.
6. \*Low-energy excitations and ground-state selection in the quantum breathing pyrochlore antiferromagnet  $\text{Ba}_3\text{Yb}_2\text{Zn}_5\text{O}_{11}$ : T. Haku, K. Kimura, Y. Matsumoto, M. Soda, M. Sera, D. Yu, R. A. Mole, T. Takeuchi, S. Nakatsuji, Y. Kono, T. Sakakibara, L. -J. Chang and T. Masuda, *Phys. Rev. B* **93** (2016) 220407(1-5).
7. Quadrupole-driven non-Fermi-liquid and magnetic-field-induced heavy fermion states in a non-Kramers doublet system: T. Onimaru, K. Izawa, K. T. Matsumoto, T. Yoshida, Y. Machida, T. Ikeura, K. Wakiya, K. Umeo, S. Kittaka, K. Araki, T. Sakakibara and T. Takabatake, *Phys. Rev. B* **94** (2016) 075134(1-8).
8. Thermodynamic study of gap structure and pair-breaking effect by magnetic field in the heavy-fermion superconductor  $\text{CeCu}_2\text{Si}_2$ : S. Kittaka, Y. Aoki, Y. Shimura, T. Sakakibara, S. Seiro, C. Geibel, F. Steglich, Y. Tsutsumi, H. Ikeda and K. Machida, *Phys. Rev. B* **94** (2016) 054514(1-9).
9. †Unconventional  $S=2$  alternating chain realized by a metal-radical hybrid-spin approach: H. Yamaguchi, Y. Shinpuku, Y. Kono, S. Kittaka, T. Sakakibara, M. Hagiwara, T. Kawakami, K. Iwase, T. Ono and Y. Hosokoshi, *Phys. Rev. B* **93** (2016) 115145(1-7).
10. †Omnidirectional Measurements of Angle-Resolved Heat Capacity for Complete Detection of Superconducting Gap Structure in the Heavy-Fermion Antiferromagnet  $\text{UPd}_2\text{Al}_3$ : Y. Shimizu, S. Kittaka, T. Sakakibara, Y. Tsutsumi, T. Nomoto, H. Ikeda, K. Machida, Y. Homma and D. Aoki, *Phys. Rev. Lett.* **117** (2016) 037001(1-5).
11. †Quadrupole Order in the Frustrated Pyrochlore  $\text{Tb}_{2+x}\text{Ti}_{2-x}\text{O}_{7+y}$ : H. Takatsu, S. Onoda, S. Kittaka, A. Kasahara, Y. Kono, T. Sakakibara, Y. Kato, B. Fåk, J. Ollivier, J. W. Lynn, T. Taniguchi, M. Wakita and H. Kadowaki, *Phys. Rev. Lett.* **116** (2016) 217201(1-6).
12. †Comparison With Ground States of Frustrated Quantum Spin Chain Systems  $\text{A}_2\text{Cu}_2\text{Mo}_3\text{O}_{12}$  ( $A = \text{Rb}$  and  $\text{Cs}$ ): A. Fujimura, Y. Yasui, Y. Yanagisawa, I. Terasaki, Y. Kono, S. Kittaka and T. Sakakibara, *IEEE Trans. Magn.* **52** (2016) 1100503(3pages).
13. †Angle-resolved heat capacity of heavy fermion superconductors: T. Sakakibara, S. Kittaka and K. Machida, *Rep. Prog. Phys.* **79** (2016) 094002(1-19).
14. †Ferromagnetic ordered phase of quantum spin ice system  $\text{Yb}_2\text{Ti}_2\text{O}_7$  under [001] magnetic field: N. Hamachi, Y. Yasui, K. Araki, S. Kittaka and T. Sakakibara, *AIP Advances* **6** (2016) 055707(1-6).
15. †Possible observation of highly itinerant quantum magnetic monopoles in the frustrated pyrochlore  $\text{Yb}_2\text{Ti}_2\text{O}_7$ : Y. Tokiwa, T. Yamashita, M. Udagawa, S. Kittaka, T. Sakakibara, D. Terazawa, Y. Shimoyama, T. Terashima, Y. Yasui, T. Shibauchi and Y. Matsuda, *Nat. Commun.* **7** (2016) 10807(1-6).
16. †Quadrupole order in the frustrated pyrochlore magnet  $\text{Tb}_2\text{Ti}_2\text{O}_7$ : H. Takatsu, T. Taniguchi, S. Kittaka, T. Sakakibara and H. Kadowaki, *J. Phys.: Conf. Series* **683** (2016) 012022(1-6).
17. Structural, Magnetic, and Superconducting Properties of Caged Compounds  $\text{ROs}_2\text{Zn}_{20}$  ( $R = \text{La}, \text{Ce}, \text{Pr}, \text{and Nd}$ ): K. Wakiya, T. Onimaru, K. T. Matsumoto, Y. Yamane, N. Nagasawa, K. Umeo, S. Kittaka, T. Sakakibara, Y. Matsushita and T. Takabatake, *J. Phys. Soc. Jpn.* **86** (2017) 034707(1-6).
18. \*Thermodynamic Investigation of Metamagnetic Transitions and Partial Disorder in the Quasi-Kagome Kondo Lattice  $\text{CePdAl}$ : K. Mochidzuki, Y. Shimizu, A. Kondo, S. Nakamura, S. Kittaka, Y. Kono, T. Sakakibara, Y. Ikeda, Y. Isikawa and K. Kindo, *J. Phys. Soc. Jpn.* **86** (2017) 034709(1-5).
19. †Magnetic properties of the  $S=1/2$  honeycomb lattice antiferromagnet 2-Cl-3,6-F<sub>2</sub>-V: T. Okabe, H. Yamaguchi, S. Kittaka, T. Sakakibara, T. Ono and Y. Hosokoshi, *Phys. Rev. B* **95** (2017) 075120(1-6).
20. Nodal gap structure of the heavy-fermion superconductor  $\text{URu}_2\text{Si}_2$  revealed by field-angle-dependent specific-heat measurements: S. Kittaka, Y. Shimizu, T. Sakakibara, Y. Haga, E. Yamamoto, Y. Onuki, Y. Tsutsumi, T. Nomoto, H. Ikeda and K. Machida, *J. Phys.: Conf. Ser.* **807** (2017) 052001(1-6).

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† Joint research with outside partners.

21. Thermodynamic properties of quadrupolar states in the frustrated pyrochlore magnet  $Tb_2Ti_2O_7$ : H. Takatsu, T. Taniguchi, S. Kittaka, T. Sakakibara and H. Kadowaki, *J. Phys.: Conf. Ser.* **828** (2017) 012007(1-6).
22. \*Unique Electronic States in Non-centrosymmetric Cubic Compounds: M. Kakihana, K. Nishimura, Y. Ashitomi, T. Yara, D. Aoki, A. Nakamura, F. Honda, M. Nakashima, Y. Amako, Y. Uwatoko, T. Sakakibara, S. Nakamura, T. Takeuchi, Y. Haga, E. Yamamoto, H. Harima, M. Hedo, T. Nakama and Y. Onuki, *J. Electron. Mater.* **46** (2017) 3572-3586.
23. 重い電子系における超伝導研究の新展開 —磁場角度分解比熱測定からみたギャップ対称性—: 橘高俊 一郎, 榊原 俊郎, 町田 一成, *固体物理* **51** (2016) 411-427.
24. 磁場角度回転比熱測定による超伝導研究: 橘高俊 一郎, *物性研究・電子版* **6** (2017) 85-125.
25. 基礎の物性実験 - 比熱・磁化測定からわかること: 榊原 俊郎, 「物性科学ハンドブック - 概念・現象・物質 -」, 5, 家泰弘, 高田康民, (朝倉書店, 2016), 233-290.

## Mori group

We have successfully developed and unveiled unprecedented functional properties for the molecular materials. The major achievements in 2016 are (1) to disclose the chemical pressure effect by anion substitution on hydrogen-bond-mediated phase transition of  $\beta'$ - $H_3(\text{Cat-EDO-TTF})_2\text{BF}_4$ , (2) to improve the stability of a metallic state in benzothienobenzothiophene-based molecular conductor,  $\beta$ -[BTBT(OH) $_2$ ]ClO $_4$ , by an effective increase of dimensionality with hydrogen bonds, and (3) to investigate theoretically the H/D isotope effects on phase transition of hydrogen-bonded organic conductor  $\kappa$ -D $_3(\text{Cat-EDT-X})_2$  (X = TTF and ST).

1. Theoretical study of the H/D isotope effect on phase transition of hydrogen-bonded organic conductor  $\kappa$ - $H_3(\text{Cat-EDT-TTF})_2$ : K. Yamamoto, Y. Kanematsu, U. Nagashima, A. Ueda, H. Mori and M. Tachikawa, *Phys. Chem. Chem. Phys.* **18** (2016) 29673.
2. Novel electronic ferroelectricity in an organic charge-order insulator investigated with terahertz-pump optical-probe spectroscopy: H. Yamakawa, T. Miyamoto, T. Morimoto, H. Yada, Y. Kinoshita, M. Sotome, N. Kida, K. Yamamoto, K. Iwano, Y. Matsumoto, S. Watanabe, Y. Shimoi, M. Suda, H. M. Yamamoto, H. Mori and H. Okamoto, *Sci. Rep.* **6** (2016) 20571(1-10).
3. Improved stability of a metallic state in benzothienobenzothiophene-based molecular conductors: an effective increase of dimensionality with hydrogen bonds: T. Higashino, A. Ueda, J. Yoshida and H. Mori, *Chem. Commun.* **53** (2017) 3426.
4. Anion substitution in hydrogen-bonded organic conductors: the chemical pressure effect on hydrogen-bond-mediated phase transition: J. Yoshida, A. Ueda, R. Kumai, Y. Murakami and H. Mori, *CrystEngComm* **19** (2017) 367.
5. Valence engineering of ionic molecular crystals: monovalent–divalent phase diagram for biferrocene–tetracyanoquinodimethane salts: T. Mochida, Y. Funasako, T. Akasaka, M. Uruichi and H. Mori, *CrystEngComm* **19** (2017) 1449.
6. Multicomponent DFT study of geometrical H/D isotope effect on hydrogen-bonded organic conductor,  $\kappa$ - $H_3(\text{Cat-EDT-ST})_2$ : K. Yamamoto, Y. Kanematsu, U. Nagashima, A. Ueda, H. Mori and M. Tachikawa, *Chemical Physics Letters* **674** (2017) 168.
7. 水素結合- $\pi$ 電子系相関型有機伝導体の開発とその水素重水素同位体効果: 上田 顕, 森 初果, *J. Comput. Chem. Jpn* **15** (2016) 163-169.

## Osada group

We have studied the transport properties of the high-mobility thin-film black phosphorus (BP) field effect transistor (FET) device, and have newly found double carrier transport features in positively gated (electron-doped) region. We built a van der Waals stacking structure, hexagonal boron nitride (h-BN)/thin-film PB (15-20 nm)/h-BN on  $\text{SiO}_2/n^+\text{-Si}$  substrate, in the groove box environment and then fabricated it into an FET device. By avoiding the degradation of BP by oxygen and water using the h-BN sandwiched structure, the carrier mobility in the FET has reached 6,000  $\text{cm}^2/\text{Vs}$  for holes and 5,800  $\text{cm}^2/\text{Vs}$  for electrons, which are the highest mobility ever reported. We have newly observed double period Shubnikov-de Haas oscillations, which indicates two Fermi surfaces (FSs), in the highly electron doped region (positively gated region). The second FS is considered to originate from the second electron subband in the ultra-thin BP films.

1. 原子層におけるトポロジ物理学: 長田 俊人, *表面科学* **37** (2016) 535-540.

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\* Joint research among groups within ISSP.

2. 「物性科学ハンドブック - 概念・現象・物質 -」(東京大学物性研究所 編) 第7章「電気伝導 - 低次元電子系の量子伝導」: 長田 俊人, (朝倉書店, 東京, 2016).

## Yamashita group

We have been studying (1) quantum criticality in heavy-fermion materials by ultra-low temperature cryostat, (2) thermal-Hall conductivity of exotic excitations in frustrated magnets and (3) a new technique for the study of strongly-correlated electron systems. In this year, we have performed (1) Co and In NMR measurements of CeCoIn<sub>5</sub> at ultra-low temperatures, (2) thermal Hall measurements in spin liquid materials Ba<sub>3</sub>CuSb<sub>2</sub>O<sub>9</sub> and alpha-RuCl<sub>3</sub> and (3) scanning-Hall measurements of Mn<sub>3</sub>Sn.

1. \*Dome-shaped magnetic order competing with high-temperature superconductivity at high pressures in FeSe: J. P. Sun, K. Matsuura, G. Z. Ye, Y. Mizukami, M. Shimozawa, K. Matsubayashi, M. Yamashita, T. Watashige, S. Kasahara, Y. Matsuda, J. -Q. Yan, B. C. Sales, Y. Uwatoko, J. -G. Cheng and T. Shibauchi, *Nat. Commun.* **7** (2016) 12146(1-15).
2. \*Emergence of nontrivial magnetic excitations in a spin-liquid state of kagomé volborthite: D. Watanabe, K. Sugii, M. Shimozawa, Y. Suzuki, T. Yajima, H. Ishikawa, Z. Hiroi, T. Shibauchi, Y. Matsuda and M. Yamashita, *Proc. Natl. Acad. Sci. U.S.A.* **113** (2016) 8653.
3. \*Thermal Hall Effect in a Phonon-Glass Ba<sub>3</sub>CuSb<sub>2</sub>O<sub>9</sub>: K. Sugii, M. Shimozawa, D. Watanabe, Y. Suzuki, M. Halim, M. Kimata, Y. Matsumoto, S. Nakatsuji and M. Yamashita, *Phys. Rev. Lett.* **118** (2017) 145902.

## Division of Condensed Matter Theory

### Tsunetsugu group

We have completed the study of optical conductivity near antiferromagnetic transition. The main result is the importance of vertex corrections, and this is different from the case of Mott transition, where the vertex corrections have little effects. We also completed the study of quadrupole antiferro orders in a heavy fermion system, and determined the detailed phase diagram in temperature and magnetic field space. Spin singlet order in breathing pyrochlores has been also investigated in detail, and we have found that the spin size essentially change a ground state order. For  $S > 1/2$ , tetramer orders are stabilized, which contrasts to dimer orders in the  $S = 1/2$  case. For this problem, we have developed a systematic scheme of degenerate perturbation tailored for breathing pyrochlores, and derived an effective Hamiltonian for low-energy dynamics.

1. Classical Monte Carlo Study for Antiferro Quadrupole Orders in a Diamond Lattice: K. Hattori and H. Tsunetsugu, *J. Phys. Soc. Jpn.* **85** (2016) 094001(1-14).
2. Cluster dynamical mean field theory study of antiferromagnetic transition in the square-lattice Hubbard model: Optical conductivity and electronic structure: T. Sato and H. Tsunetsugu, *Phys. Rev. B* **94** (2016) 085110(1-12).
3. Entanglement prethermalization in an interaction quench between two harmonic oscillators: T. N. Ikeda, T. Mori, E. Kaminishi and M. Ueda, *Phys. Rev. E* **95** (2017) 022129(1-8).
4. Theory of antiferromagnetic Heisenberg spins on a breathing pyrochlore lattice: H. Tsunetsugu, *Prog. Theor. Exp. Phys.* **2017** (2017) 033101(1-29).

### Kato group

The main research subject of our laboratory is theory of non-equilibrium properties in nanoscale devices. We have studied (1) adiabatic pumping via a quantum dot with Coulomb interaction, (2) current fluctuations in a Kondo-correlated quantum dot, and (3) Andreev bound states in a multi-terminal superconducting device. We have also collaborated with experimentalists in ISSP, and have supported theoretical aspects on (4) pressure dependence of the magnetic ground states in MnP and (5) proximity effect at a single atomic step by STM.

1. Field-Enhanced Kondo Correlations in a Half-Filling Nanotube Dot: Evolution of an  $SU(N)$  Fermi-Liquid Fixed Point: Y. Teratani, R. Sakano, R. Fujiwara, T. Hata, T. Arakawa, M. Ferrier, K. Kobayashi and A. Oguri, *J. Phys. Soc. Jpn.* **85** (2016) 094718.
2. Order, disorder, and tunable gaps in the spectrum of Andreev bound states in a multiterminal superconducting device: T. Yokoyama, J. Reutlinger, W. Belzig and Y. V. Nazarov, *Phys. Rev. B* **95** (2016) 045411.

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† Joint research with outside partners.

3. \* Pressure dependence of the magnetic ground states in MnP: M. Matsuda, F. Ye, S. E. Dissanayake, J. -G. Cheng, S. Chi, J. Ma, H. D. Zhou, J. -Q. Yan, S. Kasamatsu, O. Sugino, T. Kato, K. Matsubayashi, T. Okada and Y. Uwatoko, *Phys. Rev. B* **93** (2016) 100405(1-5).
4. \* Electrical Conductivity through a Single Atomic Step Measured with the Proximity-Induced Superconducting Pair Correlation: H. Kim, S.-Z. Lin, M. J. Graf, Y. Miyata, Y. Nagai, T. Kato and Y. Hasegawa, *Phys. Rev. Lett.* **117** (2016) 116802(1-5).
5. Temperature-Driven and Electrochemical-Potential-Driven Adiabatic Pumping via a Quantum Dot: M. Hasegawa and T. Kato, *J. Phys. Soc. Jpn.* **86** (2017) 024710.
6. Quantum Fluctuations along Symmetry Crossover in a Kondo-Correlated Quantum Dot: M. Ferrier, T. Arakawa, T. Hata, R. Fujiwara, R. Delagrange, R. Deblock, Y. Teratani, R. Sakano, A. Oguri and K. Kobayashi, *Phys. Rev. Lett.* **118** (2017) 196803.

## Division of Nanoscale Science

### Katsumoto group

We have continued the study of the proximity superconductivity in a ferromagnetic semiconductor (In,Fe)As. The hysteretic behavior of the critical current indicates that the spin-triplet type pairing is realized inside (In,Fe)As. On the other hand, a Heusler ferromagnet Co<sub>2</sub>FeSi does not show any proximity superconductivity probably due to the clean ferromagnet-superconductor interface. Microwave response of two-dimensional electrons in quantum Hall state has been studied. By applying gate voltage and controlling the effective sample edge, previously-found absorption peaks are greatly enhanced, which result manifest that the peaks correspond to the edge plasmon absorption.

1. Introduction of Spin–Orbit Interaction into Graphene with Hydrogenation: T. Nakamura, J. Haruyama and S. Katsumoto, *J. Phys. Soc. Jpn.* **85** (2016) 105002.
2. Spin polarization in the vicinity of quantum point contact with spin-orbit interaction: S. Kim, Y. Hashimoto, T. Nakamura and S. Katsumoto, *Phys. Rev. B* **94** (2016) 125307.
3. †Gate-Tunable Atomically Thin Lateral MoS<sub>2</sub> Schottky Junction Patterned by Electron Beam: Y. Katagiri, T. Nakamura, A. Ishii, C. Ohata, M. Hasegawa, S. Katsumoto, T. Cusati, A. Fortunelli, G. Iannaccone, G. Fiori, S. Roche and J. Haruyama, *Nano Lett.* **16** (2016) 3788-3794.
4. Spin phase protection in interference of electron spin waves in lightly hydrogenated graphene: T. Kato, J. Kamijo, T. Nakamura, C. Ohata, S. Katsumoto and J. Haruyama, *RSC Adv.* **6** (2016) 67586.
5. †Photoresponse in gate-tunable atomically thin lateral MoS<sub>2</sub> Schottky junction patterned by electron beam: Y. Katagiri, T. Nakamura, C. Ohata, S. Katsumoto and J. Haruyama, *Appl. Phys. Lett.* **110** (2017) 143109.
6. Two-carrier model on the magnetotransport of epitaxial graphene containing coexisting single-layer and bilayer areas: A. Endo, J. Bao, W. Norimatsu, M. Kusunoki, S. Katsumoto and Y. Iye, *Philos. Mag.* **97** (2017) 1.
7. †Large edge magnetism in oxidized few-layer black phosphorus nanomeshes: Y. Nakanishi, A. Ishi, C. Ohata, D. Soriano, R. Iwaki, K. Nomura, M. Hasegawa, T. Nakamura, S. Katsumoto, S. Roche and J. Haruyama, *Nano Res.* **10** (2017) 718-728.

### Otani group

This year we tried to expand our research activities toward spintronics utilizing more complex materials in collaboration with the groups working on strongly correlated materials. For example, we have demonstrated magneto-chiral nonreciprocity of volume spin wave propagation in chiral-lattice ferromagnets and spin/charge interconversion using the surface state of topological insulator. We also examined systematically conventional spin Hall effects in Pt as a function of conductivity and found that the spin Hall effect of Pt is tunable. Apart from those, we newly found metal/Bi oxide interface provides an effective spin momentum locking behavior which can be applied for detection of spin currents.

1. Optimization of spin injection and spin detection in lateral nanostructures by geometrical means: O. Stejskal, J. Hamrle, J. Pištora and Y. Otani, *J. Magn. Magn. Mater.* **414** (2016) 132.

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\* Joint research among groups within ISSP.

2. Magnetochiral nonreciprocity of volume spin wave propagation in chiral-lattice ferromagnets: S. Seki, Y. Okamura, K. Kondou, K. Shibata, M. Kubota, R. Takagi, F. Kagawa, M. Kawasaki, G. Tatara, Y. Otani and Y. Tokura, *Phys. Rev. B* **93** (2016) 235131.
3. Tuning the spin Hall effect of Pt from the moderately dirty to the superclean regime: E. Sagasta, Y. Omori, M. Isasa, M. Gradhand, L. E. Hueso, Y. Niimi, Y. Otani and F. Casanova, *Phys. Rev. B* **94** (2016) 060412(R).
4. Large magnetoresistance in Heusler-alloy-based epitaxial magnetic junctions with semiconducting  $\text{Cu}(\text{In}_{0.8}\text{Ga}_{0.2})\text{Se}_2$  spacer: S. Kasai, Y. K. Takahashi, P. -H. Cheng, I. Ikhtiar, T. Ohkubo, K. Kondou, Y. Otani, S. Mitani and K. Hono, *Appl. Phys. Lett.* **109** (2016) 032409.
5. Observation of anisotropic energy transfer in magnetically coupled magnetic vortex pair: N. Hasegawa, S. Sugimoto, D. Kumar, S. Barman, A. Barman, K. Kondou and Y. Otani, *Appl. Phys. Lett.* **108** (2016) 242402.
6. Spin-current-driven thermoelectric generation based on interfacial spin-orbit coupling: A. Yagmur, S. Karube, K. Uchida, K. Kondou, R. Iguchi, T. Kikkawa, Y. Otani and E. Saitoh, *Appl. Phys. Lett.* **108** (2016) 242409.
7. Experimental observation of spin-to-charge current conversion at non-magnetic metal/ $\text{Bi}_2\text{O}_3$  interfaces: S. Karube, K. Kondou and Y. Otani, *Appl. Phys. Express* **9** (2016) 033001.
8. Influence of inverse spin Hall effect in spin-torque ferromagnetic resonance measurements: K. Kondou, H. Sukegawa, S. Kasai, S. Mitani, Y. Niimi and Y. Otani, *Appl. Phys. Express* **9** (2016) 023002.
9. Spin mixing conductance in Cu–Ir dilute alloys: S. Takizawa, M. Kimata, Y. Omori, Y. Niimi and Y. Otani, *Appl. Phys. Express* **9** (2016) 063009.
10. Fermi-level-dependent charge-to-spin current conversion by Dirac surface states of topological insulators: K. Kondou, R. Yoshimi, A. Tsukazaki, Y. Fukuma, J. Matsuno, K. S. Takahashi, M. Kawasaki, Y. Tokura and Y. Otani, *Nature Phys.* **12** (2016) 1027.
11. Shape- and Interface-Induced Control of Spin Dynamics of Two-Dimensional Bicomponent Magnonic Crystals: S. Choudhury, S. Saha, R. Mandal, S. Barman, Y. Otani and A. Barman, *ACS Appl. Mater. Interfaces* **8** (2016) 18339.
12. Important role of magnetization precession angle measurement in inverse spin Hall effect induced by spin pumping: S. Gupta, R. Medwal, D. Kodama, K. Kondou, Y. Otani and Y. Fukuma, *Appl. Phys. Lett.* **110** (2017) 022404.
13. スピントロニクス実験のコツ - スピン流の計測 -: 近藤 浩太 , 大谷 義近 , *応用物理* **86** (2017) 139.
14. High output voltage of magnetic tunnel junctions with a  $\text{Cu}(\text{In}_{0.8}\text{Ga}_{0.2})\text{Se}_2$  semiconducting barrier with a low resistance–area product: K. Mukaiyama, S. Kasai, Y. K. Takahashi, K. Kondou, Y. Otani, S. Mitani and K. Hono, *Appl. Phys. Express* **10** (2017) 013008.
15. Spin pumping due to spin waves in magnetic vortex structure: N. Hasegawa, K. Kondou, M. Kimata and Y. Otani, *Appl. Phys. Express* **10** (2017) 053002.
16. Voltage-induced magnetization dynamics in CoFeB/MgO/CoFeB magnetic tunnel junctions: K. Miura, S. Yabuuchi, M. Yamada, M. Ichimura, B. Rana, S. Ogawa, H. Takahashi, Y. Fukuma and Y. Otani, *Sci. Rep.* **7** (2017) 42511.
17. Bias field tunable magnetic configuration and magnetization dynamics in  $\text{Ni}_{80}\text{Fe}_{20}$  nano-cross structures with varying arm length: K. Adhikari, S. Choudhury, R. Mandal, S. Barman, Y. Otani and A. Barman, *Journal of Applied Physics* **121** (2017) 043909.

## Komori group

Growth of hetero-epitaxial fcc Fe thin films is controlled by using a nanoscale strain-relief mechanism due to the substrate step edges. The lattice expansion/compression caused by the steps is directly observed in atomic-scale STM images accompanied with the local change of the surface electronic states. Ammonia synthesis reaction by atomic hydrogen on the N-adsorbed Cu surfaces was studied using STM. Presence of the clean Cu surface largely enhances the reaction probability owing to the hydrogen diffusion on the surface. Spin-direction of photoelectrons from spin-helical surface states is coherently controlled by linearly-polarized excitation laser light for the  $\text{Bi}_2\text{Se}_3$ , Bi(0001) and Bi/Ag(111) surfaces. The direction is three-dimensionally detected by a newly developed SARPES.

1. <sup>†\*</sup>One-dimensional metallic surface states of Pt-induced atomic nanowires on Ge(001): K. Yaji, S. Kim, I. Mochizuki, Y. Takeichi, Y. Ohtsubo, P. L. Fèvre, F. Bertran, A. Taleb-Ibrahimi, S. Shin and F. Komori, *J. Phys.: Condens. Matter* **28** (2016) 284001(1-9).

---

<sup>†</sup> Joint research with outside partners.

2. \* Coherent control over three-dimensional spin polarization for the spin-orbit coupled surface state of Bi<sub>2</sub>Se<sub>3</sub>: K. Kuroda, K. Yaji, M. Nakayama, A. Harasawa, Y. Ishida, S. Watanabe, C. -T. Chen, T. Kondo, F. Komori and S. Shin, *Phys. Rev. B* **94** (2016) 165162(R)(1-5).
3. \* Direct evidence of metallic bands in a monolayer boron sheet: B. Feng, J. Zhang, R.-Y. Liu, T. Iimori, C. Lian, H. Li, L. Chen, K. Wu, S. Meng, F. Komori and I. Matsuda, *Phys. Rev. B* **94** (2016) 041408(1-5).
4. † Epitaxially stabilized iron thin films via effective strain relief from steps: T. Miyamachi, S. Nakashima, S. Kim, N. Kawamura, Y. Tatetsu, Y. Gohda, S. Tsuneyuki and F. Komori, *Phys. Rev. B* **94** (2016) 045439(1-5).
5. † Graphene/SiC(0001) interface structures induced by Si intercalation and their influence on electronic properties of graphene: A. Visikovskiy, S.-I. Kimoto, T. Kajiwara, M. Yoshimura, T. Iimori, F. Komori and S. Tanaka, *Phys. Rev. B* **94** (2016) 245421(1-10).
6. \* Spin texture in type-II Weyl semimetal WTe<sub>2</sub>: B. Feng, Y.-H. Chan, Y. Feng, R.-Y. Liu, M.-Y. Chou, K. Kuroda, K. Yaji, A. Harasawa, P. Moras, A. Barinov, W. Malaeb, C. Bareille, T. Kondo, S. Shin, F. Komori, T.-C. Chiang, Y. Shi and I. Matsuda, *Phys. Rev. B* **94** (2016) 195134(1-5).
7. \* High-resolution three-dimensional spin- and angle-resolved photoelectron spectrometer using vacuum ultraviolet laser light: K. Yaji, A. Harasawa, K. Kuroda, S. Toyohisa, M. Nakayama, Y. Ishida, A. Fukushima, S. Watanabe, C. Chen, F. Komori and S. Shin, *Rev. Sci. Instrum.* **87** (2016) 053111(1-6).
8. Orbital Selectivity in Scanning Tunneling Microscopy: Distance-Dependent Tunneling Process Observed in Iron Nitride: Y. Takahashi, T. Miyamachi, K. Ienaga, N. Kawamura, A. Ernst and F. Komori, *Phys. Rev. Lett.* **116** (2016) 056802(1-5).
9. †\* Proving Nontrivial Topology of Pure Bismuth by Quantum Confinement: S. Ito, B. Feng, M. Arita, A. Takayama, R. -Y. Liu, T. Someya, W. -C. Chen, T. Iimori, H. Namatame, M. Taniguchi, C. -M. Cheng, S. -J. Tang, F. Komori, K. Kobayashi, T. -C. Chiang and I. Matsuda, *Phys. Rev. Lett.* **117** (2016) 236402(1-5).
10. †\* Spin Polarization and Texture of the Fermi Arcs in the Weyl Fermion Semimetal TaAs: S.-Y. Xu, I. Belopolski, D. S. Sanchez, M. Neupane, G. Chang, K. Yaji, Z. Yuan, C. Zhang, K. Kuroda, G. Bian, C. Guo, H. Lu, T.-R. Chang, N. Alidoust, H. Zheng, C.-C. Lee, S.-M. Huang, C.-H. Hsu, H.-T. Jeng, A. Bansil, T. Neupert, F. Komori, T. Kondo, S. Shin, H. Lin, S. Jia and M. Zahid Hasan, *Phys. Rev. Lett.* **116** (2016) 096801(1-7).
11. レーザー光励起スピン・角度分解光電子分光装置の開発: 矢治光 一郎, *表面科学* **37** (2016) 19-24.
12. Ribbon-Like Nanopattern Formed on Nitrogen-Adsorbed Vicinal Cu(001): M. Yamada, N. Kawamura, K. Nakatsuji and F. Komori, *e-J. Surf. Sci. Nanotech.* **14** (2016) 43-46.
13. \* Photoelectrochemical water splitting enhanced by self-assembled metal nanopillars embedded in an oxide semiconductor photoelectrode: S. Kawasaki, R. Takahashi, T. Yamamoto, M. Kobayashi, H. Kumigashira, J. Yoshinobu, F. Komori, A. Kudo and M. Lippmaa, *Nat. Commun.* **7** (2016) 11818(1-6).
14. † Effects of Pb Intercalation on the Structural and Electronic Properties of Epitaxial Graphene on SiC: A. Yurtsever, J. Onoda, T. Iimori, K. Niki, T. Miyamachi, M. Abe, S. Mizuno, S. Tanaka, F. Komori and Y. Sugimoto, *Small* **12** (2016) 3956–3966.
15. \* Surface state of the dual topological insulator Bi Sb (112): I. Matsuda, K. Yaji, A. A. Taskin, M. D'angelo, R. Yukawa, Y. Ohtsubo, P. Le Fèvre, F. Bertran, S. Yoshizawa, A. Taleb-Ibrahimi, A. Kakizaki, Y. Ando and F. Komori, *Physica B* **516** (2017) 100-104.
16. \* Direct mapping of spin and orbital entangled wave functions under interband spin-orbit coupling of giant Rashba spin-split surface states: R. Noguchi, K. Kuroda, K. Yaji, K. Kobayashi, M. Sakano, A. Harasawa, T. Kondo, F. Komori and S. Shin, *Phys. Rev. B* **95** (2017) 041111(R)(1-6).
17. \* Suppression of supercollision carrier cooling in high mobility graphene on SiC(000-1): T. Someya, H. Fukidome, H. Watanabe, T. Yamamoto, M. Okada, H. Suzuki, Y. Ogawa, T. Iimori, N. Ishii, T. Kanai, K. Tashima, B. Feng, S. Yamamoto, J. Itatani, F. Komori, K. Okazaki, S. Shin and I. Matsuda, *Phys. Rev. B* **95** (2017) 165303(1-7).
18. †\* Dirac Fermions in Borophene: B. Feng, O. Sugino, R.-Y. Liu, J. Zhang, R. Yukawa, M. Kawamura, T. Iimori, H. Kim, Y. Hasegawa, H. Li, L. Chen, K. Wu, H. Kumigashira, F. Komori, T.-C. Chiang, S. Meng and I. Matsuda, *Phys. Rev. Lett.* **118** (2017) 096401(1-6).
19. STM observation of the chemical reaction of atomic hydrogen on the N-adsorbed Cu(001) surface: T. Hattori, M. Yamada and F. Komori, *Surf. Sci.* **655** (2017) 1-6.

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\* Joint research among groups within ISSP.

20. \* Spin-dependent quantum interference in photoemission process from spin-orbit coupled states: K. Yaji, K. Kuroda, S. Toyohisa, A. Harasawa, Y. Ishida, S. Watanabe, C. Chen, K. Kobayashi, F. Komori and S. Shin, *Nat. Commun.* **8** (2017) 14588(1-6).
21. \* ホウ素単原子シート「ポロフェン」：金属性とディラックフェルミオン：F. Baojie, 松田 巖, *固体物理* (2017), in print.

## Hasegawa group

Using scanning tunneling microscopy (STM) we investigated transport properties of a monolayer metallic thin film formed on a semiconductor substrate using superconducting pair correlation as a probing signal. The pair correlation was induced onto the two-dimensional (2D) metallic layer by locating superconducting materials on it. Tunneling spectra taken around the proximate area provides information on how the pair correlation spread and decay from the super/normal interface and how step structures on the layer disturbs the spreading. Since these are closely related with electrical conductance, conductivity through the monoatomic layer and a atomic-high step can be estimated through the spatially resolved spectral measurements. We have taken tunneling spectra at 2.1 K around superconducting Pb island structures formed on Pb-induced striped incommensurate phase; a 2D metallic layer formed on Si(111) substrate, and obtained the conductivity through the 2D layer and across a single atomic-height step. It turned out that the steps have a significant contribution to the total resistance even on a nominally flat surface, and that macroscopic monolayer conductance, which includes the step conductance, is quite sensitive to a miscut angle of the substrate. We also demonstrate that a method of compressed sensing is quite effective to improve the quality of obtained results and to save measurement time in the observation of quasi-particle interference (QPI) by STM. Since QPI provides momentum-space information on electronic states of samples, it is a very powerful tool to investigate the electronic states at very low temperature and/or under magnetic field, where photoemission spectroscopy cannot be performed. The QPI measurement is, however, quite time-consuming; it takes a few days to a week for a single dataset. Utilizing the sparseness of the QPI signals in momentum space, we performed a sparsity-inducing algorithm called least absolute shrinkage and selection operator (LASSO), and demonstrated that LASSO recovers a circular QPI pattern of the Ag(111) surface from a dataset whose size is less than that necessary for the conventional Fourier transformation method. Our results demonstrate that the compressed sensing based on the sparse modeling works well in the QPI analysis and that the concept and the procedure should be applied to various subjects in condensed matter physics.

1. Compressed Sensing in Scanning Tunneling Microscopy/Spectroscopy for Observation of Quasi-Particle Interference: Y. Nakanishi-Ohno, M. Haze, Y. Yoshida, K. Hukushima, Y. Hasegawa and M. Okada, *J. Phys. Soc. Jpn.* **85** (2016) 093702(1-5).
2. Direct visualization of surface phase of oxygen molecules physisorbed on Ag(111) surface: A two-dimensional quantum spin system: S. Yamamoto, Y. Yoshida, H. Imada, Y. Kim and Y. Hasegawa, *Phys. Rev. B* **93** (2016) 081408(R)(1-5).
3. Insensitivity of atomic point contact conductance to a moiré structure: H. Kim and Y. Hasegawa, *Phys. Rev. B* **93** (2016) 075409(1-6).
4. Spatial variation in local work function as an origin of moiré contrast in scanning tunneling microscopy images of Pb thin films/Si(111): H. Kim and Y. Hasegawa, *Jpn. J. Appl. Phys.* **55** (2016) 08NA03(1-7).
5. \*Electrical Conductivity through a Single Atomic Step Measured with the Proximity-Induced Superconducting Pair Correlation: H. Kim, S.-Z. Lin, M. J. Graf, Y. Miyata, Y. Nagai, T. Kato and Y. Hasegawa, *Phys. Rev. Lett.* **117** (2016) 116802(1-5).
6. Superconducting proximity effect on a Rashba-split Pb/Ge(111)- $\beta\sqrt{3}\times\sqrt{3}$  surface: H. Kim, Y. Miyata and Y. Hasegawa, *Supercond. Sci. Technol.* **29** (2016) 084006(1-6).
7. Role of the substrate in the formation of chiral magnetic structures driven by the interfacial Dzyaloshinskii-Moriya interaction: M. Haze, Y. Yoshida and Y. Hasegawa, *Phys. Rev. B* **95** (2017) 060415(1-5).
8. †\*Dirac Fermions in Borophene: B. Feng, O. Sugino, R.-Y. Liu, J. Zhang, R. Yukawa, M. Kawamura, T. Iimori, H. Kim, Y. Hasegawa, H. Li, L. Chen, K. Wu, H. Kumigashira, F. Komori, T.-C. Chiang, S. Meng and I. Matsuda, *Phys. Rev. Lett.* **118** (2017) 096401(1-6).

## Lippmaa group

Our recent work is related to the materials analysis and structural design of photoelectrode materials for photoelectrochemical water splitting reactions. We have studied the process of optically excited *d*-state relaxation in oxides and discovered a relaxation path related magnetic order in MnO. This work may open a path to control the relaxation rate of excited *d*-states by external magnetic fields. Another topic is the design of self-organized nanostructures for constructing robust electrodes in oxide thin films to extract photogenerated carriers from a low-mobility oxide semiconductor. Rapid photocarrier recombination limits the maximum achievable efficiency of photoelectrochemical reactions on photoelectrode surfaces because carriers generated

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† Joint research with outside partners.



deep in the semiconductor cannot be transported to the surface without trapping and recombination. Embedding metallic nanowires in an oxide matrix helps to reduce the necessary diffusion path length for excited carriers and thus improve the efficiency of photo-induced electrochemical reactions. We have demonstrated the growth of Ir metal nanopillars in SrTiO<sub>3</sub> and showed that tubular Schottky junctions form around the nanopillars. Photocarriers generated in the Schottky depletion regions are quickly separated and transported to the film surface through the metallic nanopillars.

1. \*Optical pump-THz probe analysis of long-lived *d*-electrons and relaxation to self-trapped exciton states in MnO: J. Nishitani, T. Nagashima, M. Lippmaa and T. Suemoto, Appl. Phys. Lett. **108** (2016) 162101(1-5).
2. \*Photoexcited *d*-electron dynamics in transition metal oxide MnO studied by optical pump-THz probe measurements: J. Nishitani, T. Kurihara, A. Asahara, T. Nagashima, M. Lippmaa and T. Suemoto, Phys. Status Solidi C **13** (2016) 113-116.
3. The effect of polar (111)-oriented SrTiO<sub>3</sub> on initial perovskite growth: I. Hallsteinsen, M. Nord, T. Bolstad, P. -E. Vullum, J. E. Boschker, P. Longo, R. Takahashi, R. Holmestad, M. Lippmaa and T. Tybell, Cryst. Growth Des. **16** (2016) 2357-2362.
4. \*Photoelectrochemical water splitting enhanced by self-assembled metal nanopillars embedded in an oxide semiconductor photoelectrode: S. Kawasaki, R. Takahashi, T. Yamamoto, M. Kobayashi, H. Kumigashira, J. Yoshinobu, F. Komori, A. Kudo and M. Lippmaa, Nat. Commun. **7** (2016) 11818(1-6).
5. Superconducting coupling across a spin-filtering manganite tunnel barrier with magnetic disorder: T. Harada, M. Matvejeff, R. Takahashi and M. Lippmaa, EPL **115** (2016) 67005.
6. 自己組織的に成長する単結晶性酸化物ナノ構造の新展開—磁性体ナノ結晶とナノコンポジット水分解光電極を開発—: 高橋竜太, リップ マーミック, 固体物理 **52** (2017) 105-116.
7. Microstructure analysis of IrO<sub>2</sub> thin films: X. Hou, R. Takahashi, T. Yamamoto and M. Lippmaa, J. Cryst. Growth **462** (2017) 24-28.
8. †Combinatorial screening of halide perovskite thin films and solar cells by mask-defined IR laser molecular beam epitaxy: K. Kawashima, Y. Okamoto, O. Annayev, N. Toyokura, R. Takahashi, M. Lippmaa, K. Itaka, Y. Suzuki, N. Matsuki and H. Koinuma, Sci. Tech. Adv. Mater. **18** (2017) 307.
9. Intrinsic Superhydrophilicity of Titania-Terminated Surfaces: S. Kawasaki, E. Holmström, R. Takahashi, P. Spijker, A. S. Foster, H. Onishi and M. Lippmaa, J. Phys. Chem. C **121** (2017) 2268-2275.
10. Magnetic and Magnetodielectric Properties of Epitaxial Iron Vanadate Thin Films: D. Zhou, R. Takahashi, Y. Zhou, D. Kim, V. K. Suresh, Y.-H. Chu, Q. He, P. Munroe, M. Lippmaa, J. Seidel and N. Valanoor, Adv. Electron. Mater. **3** (2017) 1600295(1-10).
11. Thermal Stable Sr<sub>2</sub>RuO<sub>4</sub> Electrode for Oxide Heterostructures: R. Takahashi and M. Lippmaa, ACS Applied Materials & Interfaces (2017), accepted for publication.

## Functional Materials Group

### Yoshinobu group

We conducted several research projects in the fiscal year 2016. (1) The activation and hydrogenation of CO<sub>2</sub> on clean and Zn-deposited Cu(111) and Cu(997) surfaces studied by AP-XPS, IRAS, and TPD. (2) The surface chemistry of formic acid on clean and Zn-deposited Cu(111) and Cu(997) surfaces studied by SR-PES, IRAS and TPD. (3) Spectroscopic characterization of H-Cu(111), Zn-Cu(111), Pd-Cu and Pd-Ag surfaces by XPS. (4) Spectroscopic characterization of Pt atoms and clusters on graphene using SR-XPS (5) LT-STM study of CO<sub>2</sub> on Cu(997) (6) Independently driven four-probe conductivity measurement of organic thin films including pentacene etc. (7) Gas-exposure effects on single organic layer FET

1. Observation of Fano line shapes in infrared vibrational spectra of CO<sub>2</sub> adsorbed on Cu(997): T. Koitaya, Y. Shiozawa, K. Mukai, S. Yoshimoto and J. Yoshinobu, J. Chem. Phys. **144** (2016) 054703.
2. The chemistry of simple alkene molecules on Si(100)c(4x2): the mechanism of cycloaddition and their selectivities: K. Akagi and J. Yoshinobu, Surf. Sci. **652** (2016) 304-311.
3. †Mechanism of Olefin Hydrogenation Catalysis Driven by Palladium-Dissolved Hydrogen: S. Ohno, M. Wilde, K. Mukai, J. Yoshinobu and K. Fukutani, J. Phys. Chem. C **120** (2016) 11481.

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\* Joint research among groups within ISSP.

4. \* Photoelectrochemical water splitting enhanced by self-assembled metal nanopillars embedded in an oxide semiconductor photoelectrode: S. Kawasaki, R. Takahashi, T. Yamamoto, M. Kobayashi, H. Kumigashira, J. Yoshinobu, F. Komori, A. Kudo and M. Lippmaa, *Nat. Commun.* **7** (2016) 11818(1-6).
5. \* Real-time observation of reaction processes of CO<sub>2</sub> on Cu(997) by ambient-pressure X-ray photoelectron spectroscopy: T. Koitaya, S. Yamamoto, Y. Shiozawa, K. Takeuchi, R.-Y. Liu, K. Mukai, S. Yoshimoto, K. Akikubo, I. Matsuda and J. Yoshinobu, *Topic in Catalysis* **59** (2016) 526-531.
6. Electronic states and electrical conductivity of the Si(111) native oxide surface adsorbed with electron donor tetrakis(dimethylamino)ethylene: S. Yoshimoto, Y. Shiozawa, T. Koitaya, H. Noritake, K. Mukai and J. Yoshinobu, *Journal of Applied Physics* **120** (2016) 085310.
7. † Direct observation of the electron-phonon coupling between empty states in graphite via high-resolution electron energy loss spectroscopy: S.-I. Tanaka, K. Mukai and J. Yoshinobu, *Phys. Rev. B* **95** (2017) 165408.
8. \* Single-particle excitation of core states in epitaxial silicene: C.-C. Lee, J. Yoshinobu, K. Mukai, S. Yoshimoto, H. Ueda, A. Fleurence, Y. Yamada-Takamura and T. Ozaki, *Phys. Rev. B* **95** (2017) 115437.
9. \* Adsorption of CO<sub>2</sub> on Graphene: A Combined TPD, XPS, and vdW-DF Study: K. Takeuchi, S. Yamamoto, Y. Hamamoto, Y. Shiozawa, K. Tashima, H. Fukidome, T. Koitaya, K. Mukai, S. Yoshimoto, M. Suemitsu, Y. Morikawa, J. Yoshinobu and I. Matsuda, *J. Phys. Chem. C* **121** (2017) 2807.
10. \* CO<sub>2</sub> adsorption on graphene studied by TPD and DFT calculation with van der Waals density functional: K. Takeuchi, S. Yamamoto, Y. Hamamoto, Y. Shiozawa, K. Tashima, H. Fukidome, T. Koitaya, K. Mukai, S. Yoshimoto, M. Suemitsu, Y. Morikawa, J. Yoshinobu and I. Matsuda, *J. Phys. Chem. C* **121** (2017) 2807-2814.
11. † "Electronic states and growth modes of Zn atoms deposited on Cu(111) studied by XPS, UPS and DFT": T. Koitaya, Y. Shiozawa, Y. Yoshikura, K. Mukai, S. Yoshimoto, S. Torii, F. Muttaqien, Y. Hamamoto, K. Inagaki, Y. Morikawa and J. Yoshinobu, *Surface Science* **663** (2017)1-10.

## Akiyama group

In 2016, we improved accuracy of absolute electroluminescence-efficiency measurements for multi-junction solar cells by developing an integration-sphere total-flux characterization system. We started time-resolved photo-emission spectroscopy of solar cells. We studied pico- and femto-second short-pulse generation via gain switching in semiconductor lasers via optical pumping and current injection. We studied photo-cleavage and damages of caged luciferins. We made intensive studies on theoretical quantum-chemistry and molecular-dynamics calculations on oxyluciferins and related molecule systems.

1. Solar-cell radiance standard for absolute electroluminescence measurements and open-circuit voltage mapping of silicon solar modules: T. Mochizuki, C. Kim, M. Yoshita, J. Mitchell, Z. Lin, S. Chen, H. Takato, Y. Kanemitsu and H. Akiyama, *J. Appl. Phys.* **119** (2016) 034501.
2. †\* Reverse Stability of Oxyluciferin Isomers in Aqueous Solutions: Y. Noguchi, M. Hiyama, M. Shiga, O. Sugino and H. Akiyama, *J. Phys. Chem. B* **120** (2016) 8776-8783.
3. Conversion efficiency limits and bandgap designs for multi-junction solar cells with internal radiative efficiencies below unity: L. Zhu, T. Mochizuki, M. Yoshita, S. Chen, C. Kim, H. Akiyama and Y. Kanemitsu, *Opt. Express* **24** (2016) A740-A751.
4. Internal luminescence efficiencies in InGaP/GaAs/Ge triple-junction solar cells evaluated from photoluminescence through optical coupling between subcells: D. M. Tex, M. Imaizumi, H. Akiyama and Y. Kanemitsu, *Sci. Rep.* **6** (2016) 38297.
5. Sub-Cycle Optical Response Caused by Dressed State with Phase-Locked Wavefunctions: K. Uchida, T. Otobe, T. Mochizuki, C. Kim, M. Yoshita, H. Akiyama, L. N. Pfeiffer, K. W. West, K. Tanaka and H. Hirori, *Phys. Rev. Lett* **117** (2016) 277402.
6. \* High-precision group-delay dispersion measurements of optical fibers via fingerprint-spectral wavelength-to-time mapping: T. Ito, O. Slezak, M. Yoshita, H. Akiyama and Y. Kobayashi, *Photon. Res.* **4** (2016) 13-16.
7. Characterizations of Radiation Damage in Multijunction Solar Cells Focused on Subcell Internal Luminescence Quantum Yields via Absolute Electroluminescence Measurements: L. Zhu, M. Yoshita, S. Chen, T. Nakamura, T. Mochizuki, C. Kim, M. Imaizumi, Y. Kanemitsu and H. Akiyama, *IEEE J. Photovoltaics* **6** (2016) 777-782.
8. ホタル生物発光と反応経路: 樋山みやび, *IQCE\_NEWS* **036** (2016) 1.

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† Joint research with outside partners.

9. Diagnosis of GaInAs/GaAsP multiple quantum well solar cells with Bragg reflectors via absolute electroluminescence: L. Zhu, M. Yoshita, J. Tsai, Y. Wang, C. Hong, G. Chi, C. Kim, P. Yu and H. Akiyama, *IEEE Journal of Photovoltaics* **7** (2017) 781 - 786.
10. Sensitive monitoring of photocarrier densities in the active layer of a photovoltaic device with time-resolved terahertz reflection spectroscopy: G. Yamashita, E. Matsubara, M. Nagai, C. Kim, H. Akiyama, Y. Kanemitsu and M. Ashida, *Appl. Phys. Lett* **110** (2017) 071108.
11. Effect of dynamical fluctuations of hydration structures on the absorption spectra of oxyluciferin anions in aqueous solution: M. Hiyama, M. Shiga, N. Koga, O. Sugino, H. Akiyama and Y. Noguchi, *Phys. Chem. Chem. Phys* **19** (2017) 10028-10035.
12. Theoretical insights into the effect of pH values on oxidation processes in the emission of firefly luciferin in aqueous solution: M. Hiyama, H. Akiyama and N. Koga, *Luminescence* (2017), accepted for publication.
13. Accuracy Evaluations for Standardization of Multi-Junction Solar-Cell Characterizations via Absolute Electroluminescence: M. Yoshita, L. Zhu, C. Kim, H. Kubota, T. Nakamura, M. Imaizumi, Y. Kanemitsu and H. Akiyama, in: *Proceedings of the 43rd IEEE Photovoltaic Specialists Conference* (IEEE, 2016), 3570-3573.
14. Calibration standards and measurement accuracy of absolute electroluminescence and internal properties in multi-junction and arrayed solar cells: M. Yoshita, L. Zhu, C. Kim, T. Mochizuki, T. Nakamura, M. Imaizumi, S. Chen, H. Kubota, Y. Kanemitsu and H. Akiyama, in: *Proc. SPIE, Vol. 9743* (Photonics West, 2016), 97430D1-6.
15. Characterization and modeling of radiation damages via internal radiative efficiency in multi-junction solar cells: L. Zhu, M. Yoshita, T. Nakamura, M. Imaizumi, C. Kim, T. Mochizuki, S. Chen, Y. Kanemitsu and H. Akiyama, in: *Proc. SPIE, Vol. 9743* (Photonics West, 2016), 97430U1-7.
16. Current leakage and fill factor in multi-junction solar cells linked via absolute electroluminescence characterization: L. Zhu, M. Yoshita, T. Nakamura, T. Mochizuki, C. Kim, M. Imaizumi, Y. Kanemitsu and H. Akiyama, in: *Proceedings of the 43rd Photovoltaic Specialists Conference* (IEEE, 2016), 1239-1243.

## Sugino group

We have done first-principles study of materials. On the basis of the many-body Green's function method for excited states, we have developed a method for classifying excitons in a molecule which is shown particularly important for designing luminescence materials. We have also developed a wave function theory on the basis of a tensor decomposition method and, as a first step, we successfully approached a magnetic single-impurity problem. Using the density functional theory, we have studied topological materials, magnetism under high pressure, and bioluminescence.

1. †GWT + Bethe-Salpeter equation approach for photoabsorption spectra: Importance of self-consistent GW calculations in small atomic systems: R. Kuwahara, Y. Noguchi and K. Ohno, *Phys. Rev. B* **94** (2016) 121116.
2. \* Pressure dependence of the magnetic ground states in MnP: M. Matsuda, F. Ye, S. E. Dissanayake, J. -G. Cheng, S. Chi, J. Ma, H. D. Zhou, J. -Q. Yan, S. Kasamatsu, O. Sugino, T. Kato, K. Matsubayashi, T. Okada and Y. Uwatoko, *Phys. Rev. B* **93** (2016) 100405(1-5).
3. †\* Reverse Stability of Oxyluciferin Isomers in Aqueous Solutions: Y. Noguchi, M. Hiyama, M. Shiga, O. Sugino and H. Akiyama, *J. Phys. Chem. B* **120** (2016) 8776-8783.
4. Four-body correlation embedded in antisymmetrized geminal power wave function: A. Kawasaki and O. Sugino, *J. Chem. Phys.* **145** (2016) 244110.
5. † Emergence of Negative Capacitance in Multidomain Ferroelectric-Paraelectric Nanocapacitors at Finite Bias: S. Kasamatsu, S. Watanabe, C. S. Hwang and S. Han, *Adv. Mater.* **28** (2016) 335.
6. Physical Model at the Electrode-Electrolyte Interface: O. Sugino, *Lecture Notes in Energy* **32** (2016) 93.
7. † Erratum: Improved modeling of electrified interfaces using the effective screening medium method [*Phys. Rev. B* **88**, 155427 (2013)]: I. Hamada, O. Sugino, N. Bonnet and M. Otani, *Phys. Rev. B* **95** (2017) 119901.
8. †\* Dirac Fermions in Borophene: B. Feng, O. Sugino, R.-Y. Liu, J. Zhang, R. Yukawa, M. Kawamura, T. Iimori, H. Kim, Y. Hasegawa, H. Li, L. Chen, K. Wu, H. Kumigashira, F. Komori, T.-C. Chiang, S. Meng and I. Matsuda, *Phys. Rev. Lett.* **118** (2017) 096401(1-6).
9. Molecular size insensitivity of optical gap of [n] cycloparaphenylenes (n= 3-16): Y. Noguchi and O. Sugino, *J. Chem. Phys.* **146** (2017) 144304.

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\* Joint research among groups within ISSP.

10. Quantitative characterization of exciton from *GW* +Bethe-Salpeter calculation: D. Hirose, Y. Noguchi and O. Sugino, *J. Chem. Phys.* **146** (2017) 044303.
11. \* ホウ素単原子シート「ポロフェン」：金属性とディラックフェルミオン：F. Baojie, 松田 巖, *固体物理* (2017), in print.

## Quantum Materials Group

### Oshikawa group

We studied a wide range of problems in quantum condensed matter theory. In particular, we have proposed a new possibility of realizing and designing Kitaev spin liquid in materials, using Metal-Organic Frameworks. Kitaev discovered a remarkable exactly solvable spin model, which has an exotic spin liquid state as the ground state. With its bond-dependent Ising interaction, initially it was regarded as just a theoretical toy model. This perception was changed by Jackeli and Khaliullin, who found that such interactions can naturally arise from spin-orbit interaction in iridates. This led to a flurry of attempts of experimental realization of Kitaev spin liquid in iridates and  $\text{RbCl}_3$ . However, unfortunately, in these materials a sizable Heisenberg antiferromagnetic interaction arises from the direct exchange, resulting in a non-spin liquid ground state. We proposed a novel strategy of using Metal-Organic Frameworks to realize Kitaev spin liquid, and gave supporting theoretical evidences. While it is also based on Jackeli-Khaliullin mechanism, it has advantages in a natural suppression of direct exchanges and in its flexibility and tunability. In particular, it can lead to realization of a variety of three-dimensional Kitaev spin liquids.

1. †First-principles design of a half-filled flat band of the kagome lattice in two-dimensional metal-organic frameworks: M. G. Yamada, T. Soejima, N. Tsuji, D. Hirai, M. Dinca and H. Aoki, *Phys. Rev. B* **94** (2016) 081102(R).
2. †Flux quench in a system of interacting spinless fermions in one dimension: Y. O. Nakagawa, G. Misguich and M. Oshikawa, *Phys. Rev. B* **93** (2016) 174310.
3. †Magnetism and superconductivity in ferromagnetic heavy-fermion system  $\text{UCoGe}$  under in-plane magnetic fields: Y. Tada, S. Takayoshi and S. Fujimoto, *Phys. Rev. B* **93** (2016) 174512(1-7).
4. †Plaquette order in the  $\text{SU}(6)$  Heisenberg model on the honeycomb lattice: P. Nataf, M. Lajkó, P. Corboz, A. M. Läuchli, K. Penc and F. Mila, *Phys. Rev. B* **93** (2016) 201113(R)(1-6).
5. Fractional quantum Hall states of dipolar fermions in a strained optical lattice: H. Fujita, Y. O. Nakagawa, Y. Ashida and S. Furukawa, *Phys. Rev. A* **94** (2016) 043641.
6. Spin gravitational resonance and graviton detection: J. Q. Quach, *Phys. Rev. D* **93** (2016) 104048(1-6).
7. Field-free, spin-current control of magnetization in non-collinear chiral antiferromagnets: H. Fujita, *Phys. Status Solidi RRL* **11** (2016) 1600360.
8. †Magnetism in f-electron superlattices: R. Peters, Y. Tada and N. Kawakami, *Physical Review B* **94** (2016) 205142(1-6).
9. †Two No-Go Theorems on Superconductivity: Y. Tada and T. Koma, *Journal of Statistical Physics* **165** (2016) 455-470.
10. †Finite-size scaling of the Shannon-Rényi entropy in two-dimensional systems with spontaneously broken continuous symmetry: G. Misguich, V. Pasquier and M. Oshikawa, *Phys. Rev. B* **95** (2017) 195161.
11. †Symmetry Protection of Critical Phases and a Global Anomaly in 1+1 Dimensions: S. C. Furuya and M. Oshikawa, *Phys. Rev. Lett.* **118** (2017) 021601.
12. Ultrafast generation of skyrmionic defects with vortex beams: Printing laser profiles on magnets: H. Fujita and M. Sato, *Physical Review B* **95** (2017) 054421.
13. 量子異常と物性物理 (特集 物理科学, この1年) - (素粒子物理): 押川 正毅, *パリティ* **31** (2016) 43-45.
14. 物性物理と場の量子論 ～場の量子論が明かす双対性～: 押川 正毅, *数理科学* **633** (2016) 41-46.
15. †遠方見聞録: 山田 昌彦, 「東京大学理学系研究科・理学部ニュース 2016年9月号」, 理学系研究科広報委員会所属広報誌編集委員会, (東京大学大学院理学系研究科・理学部, 2016), 7-7.

### Nakatsuji group

Our group explores novel quantum phases and phase transitions in rare-earth and transition metal based compounds. The

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† Joint research with outside partners.

followings are some relevant results obtained in 2016. (1) We discovered second example of an antiferromagnet that exhibits the anomalous Hall effect at room temperature, the chiral antiferromagnet Mn<sub>3</sub>Ge. (2) The quantum criticality at ambient pressure in β-YbAlB<sub>4</sub> can be transformed into a magnetic state whose transition temperature reaches a record high value exceeding 30 K. (3) Our thermodynamic and μSR studies have revealed highly frustrated magnetism with significant quantum fluctuations in the Heisenberg spinel antiferromagnet CdYb<sub>2</sub>S<sub>4</sub>. (4) Our neutron diffraction experiments in collaboration has revealed that disorder in the pyrochlore lattice plays an important role to enhance quantum fluctuations to stabilize a quantum Coulombic phase formed in a quantum spin ice candidate Pr<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub>.

1. Multiband electronic transport in α-Yb<sub>1-x</sub>Sr<sub>x</sub>AlB<sub>4</sub>[x=0, 0.19(3)] single crystals: H. Ryu, M. Abeykoon, E. Bozin, Y. Matsumoto, S. Nakatsuji and C. Petrovic, *J. Phys.: Condens. Matter* **28** (2016) 425602.
2. \*NMR Observation of Ferro-Quadrupole Order in PrTi<sub>2</sub>Al<sub>20</sub>: T. Taniguchi, M. Yoshida, H. Takeda, M. Takigawa, M. Tsujimoto, A. Sakai, Y. Matsumoto and S. Nakatsuji, *J. Phys. Soc. Jpn.* **85** (2016) 113703(1-4).
3. Pressure-Induced Local Structural Changes in Heavy Fermion β-YbAlB<sub>4</sub>: Y. Sakaguchi, S. Ikeda, K. Kuga, S. Suzuki, S. Nakatsuji, N. Hirao, Y. Ohishi and H. Kobayashi, *J. Phys. Soc. Jpn.* **85** (2016) 023602.
4. Strong orbital fluctuations in multipolar ordered states of PrV<sub>2</sub>Al<sub>20</sub>: Y. Matsumoto, M. Tsujimoto, T. Tomita, A. Sakai and S. Nakatsuji, *J. Magn. Magn. Mater.* **400** (2016) 66.
5. Chemical and orbital fluctuations in Ba<sub>3</sub>CuSb<sub>2</sub>O<sub>9</sub>: Y. Wakabayashi, D. Nakajima, Y. Ishiguro, K. Kimura, T. Kimura, S. Tsutsui, A. Q. R. Baron, K. Hayashi, N. Happo, S. Hosokawa, K. Ohwada and S. Nakatsuji, *Phys. Rev. B* **93** (2016) 245117.
6. Collective versus local Jahn-Teller distortion in Ba<sub>3</sub>CuS<sub>2</sub>O<sub>9</sub>: Raman scattering study: N. Drichko, C. Broholm, K. Kimura, R. Ishii and S. Nakatsuji, *Phys. Rev. B* **93** (2016) 184425(1-7).
7. Field-induced quadrupolar quantum criticality in PrV<sub>2</sub>Al<sub>20</sub>: Y. Shimura, M. Tsujimoto, B. Zeng, L. Balicas, A. Sakai and S. Nakatsuji, *Phys. Rev. B* **91** (2016) 241102(1-5).
8. \*Low-energy excitations and ground-state selection in the quantum breathing pyrochlore antiferromagnet Ba<sub>3</sub>Yb<sub>2</sub>Zn<sub>5</sub>O<sub>11</sub>: T. Haku, K. Kimura, Y. Matsumoto, M. Soda, M. Sera, D. Yu, R. A. Mole, T. Takeuchi, S. Nakatsuji, Y. Kono, T. Sakakibara, L. -J. Chang and T. Masuda, *Phys. Rev. B* **93** (2016) 220407(1-5).
9. Quantum criticality and inhomogeneous magnetic order in Fe-doped α-YbAlB<sub>4</sub>: D. E. MacLaughlin, K. Kuga, L. Shu, O. O. Bernal, P. -C. Ho, S. Nakatsuji, K. Huang, Z. F. Ding, C. Tan and J. Zhang, *Phys. Rev. B* **93** (2016) 214421.
10. Dimensional Reduction in Quantum Dipolar Antiferromagnets: P. Babkevich, M. Jeong, Y. Matsumoto, I. Kovacevic, A. Finco, R. Toft-Petersen, C. Ritter, M. Månsson, S. Nakatsuji and H. M. Rønnow, *Phys. Rev. Lett.* **116** (2016) 197202.
11. †\* Slater to Mott Crossover in the Metal to Insulator Transition of Nd<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub>: M. Nakayama, T. Kondo, Z. Tian, J. J. Ishikawa, M. Halim, C. Bareille, W. Malaeb, K. Kuroda, T. Tomita, S. Ideta, K. Tanaka, M. Matsunami, S. Kimura, N. Inami, K. Ono, H. Kumigashira, L. Balents, S. Nakatsuji and S. Shin, *Phys. Rev. Lett.* **117** (2016) 05640(1-6).
12. Large anomalous Hall effect in a non-collinear antiferromagnet at room temperature: S. Nakatsuji, N. Kiyohara and T. Higo, *Nature* **527** (2016) 212-215.
13. \*Experimental exploration of novel semimetal state in strong anisotropic Pyrochlore iridate Nd<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub> under high magnetic field: Z. M. Tian, Y. Kohama, T. Tomita, J. Ishikawa, H. Mairo, K. Kindo and S. Nakatsuji, *J. Phys.: Conf. Ser.* **683** (2016) 012024(6).
14. \*Frustrated magnetism in a Mott insulator based on a transition metal chalcogenide: S. Kawamoto, T. Higo, T. Tomita, S. Suzuki, Z. M. Tian, K. Mochizuki, A. Matsuo, K. Kindo and S. Nakatsuji, *J. Phys.: Conf. Ser.* **683** (2016) 012025(4).
15. Heavy Fermion Superconductivity in Non-magnetic Cage Compound PrV<sub>2</sub>Al<sub>20</sub>: Y. Matsumoto, M. Tsujimoto, T. Tomita, A. Sakai and S. Nakatsuji, *J. Phys.: Conf. Ser.* **683** (2016) 012013(1-8).
16. High Magnetic Transition Temperature and Semiconductor like Transport Properties of Mn-doped α-YbAlB<sub>4</sub>: S. Suzuki, T. Tomita, Y. Shimura, K. Kuga, Y. Matsumoto and S. Nakatsuji, *J. Phys.: Conf. Ser.* **683** (2016) 012009(1-6).
17. Low-temperature thermal expansion measurements in PrV<sub>2</sub>Al<sub>20</sub>: A. Magata, Y. Matsumoto, M. Tsujimoto, T. Tomita, R. Kiichler, A. Sakai and S. Nakatsuji, *J. Phys.: Conf. Ser.* **683** (2016) 012014(1-5).
18. Magnetic and Transport Properties of Frustrated γ-MnPd alloys: T. Higo, N. Kiyohara, K. Iritani, A. A. Nugroho, T. Tomita and S. Nakatsuji, *J. Phys.: Conf. Ser.* **683** (2016) 012026(1-5).
19. \*Quantum Criticality Beneath the Superconducting Dome in β-YbAlB<sub>4</sub>: T. Tomita, K. Kuga, Y. Uwatoko and S. Nakatsuji, *J. Phys.: Conf. Ser.* **683** (2016) 012007(1-5).

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\* Joint research among groups within ISSP.

20. \* Single crystal  $^{27}\text{Al}$ -NMR study of the cubic  $\Gamma_3$  ground doublet system  $\text{PrTi}_2\text{Al}_{20}$ : T. Taniguchi, M. Yoshida, H. Takeda, M. Takigawa, M. Tsujimoto, A. Sakai, Y. Matsumoto and S. Nakatsuji, *J. Phys.: Conf. Ser.* **683** (2016) 012016(1-9).
21. \* Site-selective  $^{11}\text{B}$  NMR studies on  $\text{YbAlB}_4$ : S. Takano, M. S. Grbic, K. Kimura, M. Yoshida, M. Takigawa, E. C. T. O. Farrell, K. Kuga, S. Nakatsuji and H. Harima, *J. Phys.: Conf. Ser.* **683** (2016) 012008(1-6).
22. Very Low Temperature Magnetoresistance in the Quadrupole Ordered System  $\text{PrV}_2\text{Al}_{20}$ : Y. Shimura, M. Tsujimoto, B. Zeng, Q. Zhang, L. Balicas, A. Sakai and S. Nakatsuji, *J. Phys.: Conf. Ser.* **683** (2016) 012012(1-4).
23. Giant Anomalous Hall Effect in the Chiral Antiferromagnet  $\text{Mn}_3\text{Ge}$ : N. Kiyohara, T. Tomita and S. Nakatsuji, *Phys. Rev. Applied* **5** (2016) 064009.
24.  $\dagger$ \* Lifetime-Broadening-Suppressed X-ray Absorption Spectrum of  $\beta\text{-YbAlB}_4$  Deduced from  $\text{Yb } 3d \rightarrow 2p$  Resonant X-ray Emission Spectroscopy: N. Kawamura, N. Kanai, H. Hayashi, Y. H. Matsuda, M. Mizumaki, K. Kuga, S. Nakatsuji and S. Watanabe, *J. Phys. Soc. Jpn.* **86** (2017) 014711(1-7).
25. Lifetime-Broadening-Suppressed X-ray Absorption Spectrum of  $\beta\text{-YbAlB}_4$  Deduced from  $\text{Yb } 3d \rightarrow 2p$  Resonant X-ray Emission Spectroscopy: N. Kawamura, N. Kanai, H. Hayashi, Y. H. Matsuda, M. Mizumaki, K. Kuga, S. Nakatsuji and S. Watanabe, *J. Phys. Soc. Jpn.* **86** (2017) 014711.
26. Intact quasiparticles at an unconventional quantum critical point: M. L. Sutherland, E. C. T. O'Farrell, W. H. Toews, J. Dunn, S. K. Kuga, S. Nakatsuji, Y. Machida, K. Izawa and R. W. Hill, *Phys. Rev. B* **92** (2017) 041114(1-5).
27. Disordered Route to the Coulomb Quantum Spin Liquid: Random Transverse Fields on Spin Ice in  $\text{Pr}_2\text{Zr}_2\text{O}_7$ : J. -J. Wen, S. M. Koohpayeh, K. A. Ross, B. A. Trump, T. M. McQueen, K. Kimura, S. Nakatsuji, Y. Qiu, D. M. Pajerowski, J. R. D. Copley and C. L. Broholm, *Phys. Rev. Lett.* **118** (2017) 107206.
28. \* Thermal Hall Effect in a Phonon-Glass  $\text{Ba}_3\text{CuSb}_2\text{O}_9$ : K. Sugii, M. Shimosawa, D. Watanabe, Y. Suzuki, M. Halim, M. Kimata, Y. Matsumoto, S. Nakatsuji and M. Yamashita, *Phys. Rev. Lett.* **118** (2017) 145902.
29. 反強磁性体における巨大異常ホール効果：中辻 知，*応用物理* 第 86 卷 第 4 号 (2017) 310-314.
30. \* Orthogonal magnetization and symmetry breaking in pyrochlore iridate  $\text{Eu}_2\text{Ir}_2\text{O}_7$ : T. Liang, T. H. Hsieh, J. J. Ishikawa, S. Nakatsuji, L. Fu and N. P. Ong, *Nature Phys.* **13** (2017) 599-603.
31. Anisotropic Thermal Expansion of  $\alpha\text{-YbAlB}_4$ : Y. Matsumoto, K. Kuga, T. Tomita, R. Kuchler and S. Nakatsuji, *J. Phys.: Conf. Ser.* **807** (2017) 022005.
32. Specific heat and electrical resistivity at magnetic fields in antiferromagnetic heavy fermion  $\text{CeAl}_2$ : T. Ebihara, M. Tsuchiya, Y. Saitoh, J. Jatmika, M. Tsujimoto, Y. Shimura, Y. Matsumoto and S. Nakatsuji, *J. Phys.: Conf. Ser.* **807** (2017) 012011.
33. Large anomalous Hall effect in a non-collinear antiferromagnet at room temperature: S. Nakatsuji<sup>1</sup> and 2. Naoki Kiyohara<sup>1</sup> & Tomoya Higo<sup>1</sup>, *Macmillan Publishers Limited* **527** (2017) 212-215.
34. Frustrated magnetism in the Heisenberg pyrochlore antiferromagnets  $\text{AYb}_2\text{X}_4$  ( $A = \text{Cd, Mg, X} = \text{S, Se}$ ): T. Higo, K. Iritani, M. Halim, W. Higemoto, T. U. Ito, K. Kuga, K. Kimura and S. Nakatsuji, *Phys. Rev. B* (2017), in print.
35. \* パイロクロア型イリジウム酸化物  $\text{Nd}_2\text{Ir}_2\text{O}_7$  における磁場印加方向に敏感な金属 - 絶縁体転移：小濱 芳允，Z. Tian, 富田 崇弘，石川 洵，金道 浩一，石塚 大晃，中辻 知，*固体物理* **51** (2016) 339-355.
36. 強相関電子系の物質開発：序説：中辻 知，「物性科学ハンドブック - 概念・現象・物質」，13, 家 泰弘，高田康民，(朝倉書店，2016), 929-931.
37. 金属間化合物における強相関電子系：重い電子系：中辻 知，「物性科学ハンドブック - 概念・現象・物質」，13.3, 家 泰弘，高田康民，(朝倉書店，2016), 989-1007.

## Materials Design and Characterization Laboratory

### Hiroi group

The ferromagnetic and conducting magnetic domain walls in the all-in/all-out order of  $\text{Cd}_2\text{Os}_2\text{O}_7$  are studied. The superconductivity and multipolar phase transitions of the pyrochlore oxide  $\text{Cd}_2\text{Re}_2\text{O}_7$  are revisited. Many frustrated spin systems are studied.  $\text{CdK} [\text{CdCu}_3(\text{OH})_6(\text{NO}_3)_2 \cdot \text{H}_2\text{O}]$  is a structurally perfect kagome antiferromagnet crystallizing in the kapellasite-type. An

<sup>†</sup> Joint research with outside partners.

antiferromagnetic order accompanied by a small spontaneous magnetization that surprisingly is confined in the kagome plane sets in at  $T_N \sim 4$  K, well below the nearest-neighbor exchange interaction  $J/k_B = 45$  K. This suggests that a unique “ $q = 0$ ” type  $120^\circ$  spin structure with “negative” (downward) vector chirality, which breaks the underlying threefold rotational symmetry of the kagome lattice and thus allows a spin canting within the plane, is exceptionally realized in this compound rather than a common one with “positive” (upward) vector chirality. The origin is discussed in terms of the Dzyaloshinskii-Moriya interaction. The quasi-1D antiferromagnet  $\text{NaCuMoO}_4(\text{OH})$ , which comprises edge-sharing  $\text{CuO}_2$  chains, is shown to be a good candidate for the frustrated  $J_1$ – $J_2$  chain model with  $J_1 = 51$  K and  $J_2 = 36$  K. We are now looking for evidence of a spin nematic state expected just below the saturation field of 26 T.  $\text{AMoOPO}_4\text{Cl}$  ( $A = \text{K, Rb}$ ) with  $\text{Mo}^{5+}$  ions in the  $4d^1$  electronic configuration are good model compounds for the spin-1/2  $J_1$ – $J_2$  square-lattice magnet. Magnetic transitions are observed at around 6 and 8 K in the K and Rb compounds, respectively. In contrast to the normal Néel-type antiferromagnetic order, the NMR and neutron diffraction experiments find a columnar antiferromagnetic order for each compound, which is stabilized by a dominant antiferromagnetic  $J_2$ . Both compounds realize the unusual case of two interpenetrating  $J_2$  square lattices weakly coupled to each other by  $J_1$ .

1. †\* Pressure-induced non-superconducting phase of  $\beta\text{-Na}_{0.33}\text{V}_2\text{O}_5$  and the mechanism of high-pressure phase transitions in  $\beta\text{-Na}_{0.33}\text{V}_2\text{O}_5$  and  $\beta\text{-Li}_{0.33}\text{V}_2\text{O}_5$  at room temperature: A. Grzechnik, Y. Ueda, T. Yamauchi, M. Hanfland, P. Hering, V. Potapkin and K. Friese, *J. Phys.: Condens. Matter* **28** (2016) 035401(1-9).
2. \* Emergence of nontrivial magnetic excitations in a spin-liquid state of kagomé volborthite: D. Watanabe, K. Sugii, M. Shimozawa, Y. Suzuki, T. Yajima, H. Ishikawa, Z. Hiroi, T. Shibauchi, Y. Matsuda and M. Yamashita, *Proc. Natl. Acad. Sci. U.S.A.* **113** (2016) 8653.
3. †\* Hybrid Amine-Functionalized Graphene Oxide as a Robust Bifunctional Catalyst for Atmospheric Pressure Fixation of Carbon Dioxide using Cyclic Carbonates: V. B. Saptal, T. Sasaki, K. Harada, D. Nishio-Hamane and B. M. Bhanage, *ChemSusChem* **9** (2016) 644.
4. †\* Light and SEM observation of opal phytoliths in the mulberry leaf: O. Tsutsui, R. Sakamoto, M. Obayashi, S. Yamakawa, T. Handa, D. Nishio-Hamane and I. Matsuda, *Flora* **218** (2016) 44-50.
5. †\* Bunnoite, a new hydrous manganese aluminosilicate from Kamo Mountain, Kochi prefecture, Japan: D. Nishio-Hamane, K. Momma, R. Miyawaki and T. Minakawa, *Miner Petrol* **110** (2016) 917.
6.  $J_1$ – $J_2$  square-lattice Heisenberg antiferromagnets with  $4d^1$  spins:  $\text{AMoOPO}_4\text{Cl}$  ( $A = \text{K, Rb}$ ): H. Ishikawa, N. Nakamura, M. Yoshida, M. Takigawa, P. Babkevich, N. Qureshi, H. M. Rønnow, T. Yajima and Z. Hiroi, *Phys. Rev. B* **95** (2017) 064408.
7. \* Magnetic transitions under ultrahigh magnetic fields of up to 130 T in the breathing pyrochlore antiferromagnet  $\text{LiInCr}_4\text{O}_8$ : Y. Okamoto, D. Nakamura, A. Miyake, S. Takeyama, M. Tokunaga, A. Matsuo, K. Kindo and Z. Hiroi, *Phys. Rev. B* **95** (2017) 134438.
8. Successive spatial symmetry breaking under high pressure in the spin-orbit-coupled metal  $\text{Cd}_2\text{Re}_2\text{O}_7$ : J.-I. Yamaura, K. Takeda, Y. Ikeda, N. Hirao, Y. Ohishi, T. C. Kobayashi and Z. Hiroi, *Phys. Rev. B* **95** (2017) 020102.
9. \* Weak ferromagnetic order breaking the threefold rotational symmetry of the underlying kagome lattice in  $\text{CdCu}_3(\text{OH})_6(\text{NO}_3)_2 \cdot \text{H}_2\text{O}$ : R. Okuma, T. Yajima, D. Nishio-Hamane, T. Okubo and Z. Hiroi, *Phys. Rev. B* **95** (2017) 094427.
10. Robust ferromagnetism carried by antiferromagnetic domain walls: H. T. Hirose, J.-I. Yamaura and Z. Hiroi, *Sci. Rep.* **7** (2017) 42440.
11. \* Post-Cotunnite Phase Transition in Zirconia at High Pressure: D. Nishio-Hamane, in: *Photon Factory Highlights 2015* (KEK, 2016), 38-39.

## Kawashima group

We have been investigating quantum spin/boson systems and frustrated systems by means of large-scale numerical simulation. We also develop new numerical techniques. Our group's activities of 2016 include: (1) development of the tensor network algorithms and codes suitable for parallel computation, (2) application of the tensor network methods to frustrated spin / fermion systems, and (3) quantum Monte Carlo simulation of bosonic systems targeting the two-dimensional Helium system.

1. Clues and criteria for designing a Kitaev spin liquid revealed by thermal and spin excitations of the honeycomb iridate  $\text{Na}_2\text{IrO}_3$ : Y. Yamaji, T. Suzuki, T. Yamada, S.-I. Suga, N. Kawashima and M. Imada, *Phys. Rev. B* **93** (2016) 174425.
2. Tensor network algorithm by coarse-graining tensor renormalization on finite periodic lattices: H.-H. Zhao, Z.-Y. Xie, T. Xiang and M. Imada, *Phys. Rev. B* **93** (2016) 125115(1-14).

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\* Joint research among groups within ISSP.

- Quantum lattice model solver  $H\Phi$ : M. Kawamura, K. Yoshimi, T. Misawa, Y. Yamaji, S. Todo and N. Kawashima, *Computer Physics Communications* (2017) S0010465517301200, accepted for publication.

## Uwatoko group

Temperature dependence of resistivity on  $KFe_2As_2$  single crystals down to 20 mK was measured under various hydrostatic pressures up to 17.5 GPa generated in a cubic-anvil cell. With increasing the pressure, the superconducting transition of tetragonal  $KFe_2As_2$  was suppressed gradually and disappears completely at  $\sim 11$  GPa, which was related to the weakening of electronic correlations and/or critical fluctuations under pressure. MnP, a superconductor under pressure, exhibits a ferromagnetic order below  $T_C \sim 290$  K followed by a helical order with the spins lying in the *ab* plane and the helical rotation propagating along the *c* axis below  $T_s \sim 50$  K at ambient pressure. Both  $T_C$  and  $T_s$  are gradually suppressed with increasing pressure and the helical order disappears at  $\sim 1.2$  GPa. At intermediate pressures of 1.8 and 2.0 GPa, the ferromagnetic order first develops and changes to a conical or two-phase (ferromagnetic and helical) structure with the propagation along the *b* axis below a characteristic temperature. At 3.8 GPa, a helical magnetic order appears below 208 K, which hosts the spins in the *ac* plane and the propagation along the *b* axis. The high-pressure magnetotransport measurements in FeSe up to  $\sim 15$  GPa are reported. Above  $\sim 6$  GPa the sudden enhancement of superconductivity ( $T_C \leq 38.3$  K) accompanies a suppression of magnetic order. The obtained phase diagram highlights unique features of FeSe among iron-based superconductors. And effect of pressure on the several Eu compounds have been investigated as results of joint program.

- <sup>†</sup>Kondo Effect in  $CeX_c$  ( $X_c = S, Se, Te$ ) Studied by Electrical Resistivity Measurements under High Pressure: Y. Hayashi, S. Takai, T. Matsumura, H. Tanida, M. Sera, K. Matsubayashi, Y. Uwatoko and A. Ochiai, *J. Phys. Soc. Jpn.* **85** (2016) 034704(1-7).
- <sup>†</sup>Magnetic and Fermi Surface Properties of Ferromagnets  $EuPd_2$  and  $EuPt_2$ : A. Nakamura, H. Akamine, Y. Ashitomi, F. Honda, D. Aoki, T. Takeuchi, K. Matsubayashi, Y. Uwatoko, Y. Tatetsu, T. Maehira, M. Hedo, T. Nakama and Y. Onuki, *J. Phys. Soc. Jpn.* **85** (2016) 084705.
- <sup>†</sup>Superconducting and Fermi Surface Properties of Single Crystal  $Zr_2Co$ : A. Teruya, M. Kakihana, T. Takeuchi, D. Aoki, F. Honda, A. Nakamura, Y. Haga, K. Matsubayashi, Y. Uwatoko, H. Harima, M. Hedo, T. Nakama and Y. Onuki, *J. Phys. Soc. Jpn.* **85** (2016) 034706(1-10).
- Absence of superconductivity in the collapsed tetragonal phase of  $KFe_2As_2$  under hydrostatic pressure: B. Wang, K. Matsubayashi, J. Cheng, T. Terashima, K. Kihou, S. Ishida, C.-H. Lee, A. Iyo, H. Eisaki and Y. Uwatoko, *Phys. Rev. B* **94** (2016) 020502(1-5).
- Anomalous bulk modulus in vanadate spinels: Z. -Y. Li, X. Li, J. -G. Cheng, L. G. Marshall, X. -Y. Li, A. M. dos Santos, W. -G. Yang, J. J. Wu, J. -F. Lin, G. Henkelman, T. Okada, Y. Uwatoko, H. B. Cao, H. D. Zhou, J. B. Goodenough and J. -S. Zhou, *Phys. Rev. B* **94** (2016) 165159(1-10).
- Competition of superconductivity with the structural transition in  $Mo_3Sb_7$ : G. Z. Ye, J. -G. Cheng, J. -Q. Yan, J. P. Sun, K. Matsubayashi, T. Yamauchi, T. Okada, Q. Zhou, D. S. Parker, B. C. Sales and Y. Uwatoko, *Phys. Rev. B* **94** (2016) 224508(1-7).
- Long-range magnetic order in the Heisenberg pyrochlore antiferromagnets  $Gd_2Ge_2O_7$  and  $Gd_2Pt_2O_7$  synthesized under high pressure: X. Li, Y. Q. Cai, Q. Cui, C. J. Lin, Z. L. Dun, K. Matsubayashi, Y. Uwatoko, Y. Sato, T. Kawae, S. J. Lv, C. Q. Jin, J. -S. Zhou, J. B. Goodenough, H. D. Zhou and J. -G. Cheng, *Phys. Rev. B* **94** (2016) 214429(1-9).
- \* Pressure dependence of the magnetic ground states in MnP: M. Matsuda, F. Ye, S. E. Dissanayake, J. -G. Cheng, S. Chi, J. Ma, H. D. Zhou, J. -Q. Yan, S. Kasamatsu, O. Sugino, T. Kato, K. Matsubayashi, T. Okada and Y. Uwatoko, *Phys. Rev. B* **93** (2016) 100405(1-5).
- Magnetic Precursor of the Pressure-Induced Superconductivity in Fe-Ladder Compounds: S. Chi, Y. Uwatoko, H. Cao, Y. Hirata, K. Hashizume, T. Aoyama and K. Ohgushi, *Phys. Rev. Lett.* **117** (2016) 047003(1-5).
- Slater Insulator in Iridate Perovskites with Strong Spin-Orbit Coupling: Q. Cui, J. -G. Cheng, W. Fan, A. E. Taylor, S. Calder, M. A. McGuire, I.-Q. Yan, D. Meyers, X. Li, Y. Q. Cai, Y. Y. Jiao, Y. Choi, D. Haskel, H. Gotou, Y. Uwatoko, J. Chakhalian and A. D. Christianson, *Phys. Rev. Lett.* **117** (2016) 176603.
- \* Quantum Criticality Beneath the Superconducting Dome in  $\beta$ - $YbAlB_4$ : T. Tomita, K. Kuga, Y. Uwatoko and S. Nakatsuji, *J. Phys.: Conf. Ser.* **683** (2016) 012007(1-5).
- \* Dome-shaped magnetic order competing with high-temperature superconductivity at high pressures in FeSe: J. P. Sun, K. Matsuura, G. Z. Ye, Y. Mizukami, M. Shimozawa, K. Matsubayashi, M. Yamashita, T. Watashige, S. Kasahara, Y. Matsuda, J. -Q. Yan, B. C. Sales, Y. Uwatoko, J. -G. Cheng and T. Shibauchi, *Nat. Commun.* **7** (2016) 12146(1-15).

<sup>†</sup> Joint research with outside partners.



13. Iron arsenides with three-dimensional FeAs layer networks:  $\text{Ca}_{n(n+1)/2}(\text{Fe}_{1-x}\text{Pt}_x)_{(2+3n)}\text{Pt}_{n(n-1)/2}\text{As}_{(n+1)(n+2)/2}$  ( $n=2,3$ ): N. Katayama, S. Onari, K. Matsubayashi, Y. Uwatoko and H. Sawa, *Sci. Rep.* **6** (2016) 39280(1-5).
14. † Conducting Behavior and Valence Ordering of a One-Dimensional MMX-Type Coordination Polymer under High Pressure: K. Otsubo, T. Suto, A. Kobayashi, R. Ikeda, M. Hedo, Y. Uwatoko and H. Kitagawa, *Eur. J. Inorg. Chem.* **2016** (2016) 4402-4407.
15. † Magnetic and Structural Properties of Metamagnetic  $\text{MnCo}_{0.92}\text{Fe}_{0.08}\text{Ge}$  Compound: K. Ozono, Y. Mitsui, M. Hiroi, R. Y. Umetsu, K. Takahashi, K. Matsubayashi, Y. Uwatoko and K. Koyama, *MATERIALS TRANSACTIONS* **57** (2016) 316-320.
16. † Pressure-Induced Metallization in Iron-Based Ladder Compounds  $\text{Ba}_{1-x}\text{Cs}_x\text{Fe}_2\text{Se}_3$ : T. Hawaii, C. Kawashima, K. Ohgushi, K. Matsubayashi, Y. Nambu, Y. Uwatoko, T. J. Sato and H. Takahashi, *J. Phys. Soc. Jpn.* **86** (2017) 024701(1-4).
17. † Unique Pressure versus Temperature Phase Diagram for Antiferromagnets  $\text{Eu}_2\text{Ni}_3\text{Ge}_5$  and  $\text{EuRhSi}_3$ : M. Nakashima, Y. Amako, K. Matsubayashi, Y. Uwatoko, M. Nada, K. Sugiyama, M. Hagiwara, Y. Haga, T. Takeuchi, A. Nakamura, H. Akamine, K. Tomori, T. Yara, Y. Ashitomi, M. Hedo, T. Nakama and Y. Onuki, *J. Phys. Soc. Jpn.* **86** (2017) 034708(1-13).
18. \* Two-carrier analyses of the transport properties of black phosphorus under pressure: K. Akiba, A. Miyake, Y. Akahama, K. Matsubayashi, Y. Uwatoko and M. Tokunaga, *Phys. Rev. B* **95** (2017) 115126(1-7).
19. † Superconducting, Fermi surface, and magnetic properties in  $\text{SrTGe}_3$  and  $\text{EuTGe}_3$  (T: transition metal) with the Rashba-type tetragonal structure: M. Kakihana, H. Akamine, K. Tomori, K. Nishimura, A. Teruya, A. Nakamura, F. Honda, D. Aoki, M. Nakashima, Y. Amako, K. Matsubayashi, Y. Uwatoko, T. Takeuchi, T. Kida, M. Hagiwara, Y. Haga, E. Yamamoto, H. Harima, M. Hedo, T. Nakama and Y. Onuki, *J. Alloys Compd.* **694** (2017) 439-451.
20. \* Unique Electronic States in Non-centrosymmetric Cubic Compounds: M. Kakihana, K. Nishimura, Y. Ashitomi, T. Yara, D. Aoki, A. Nakamura, F. Honda, M. Nakashima, Y. Amako, Y. Uwatoko, T. Sakakibara, S. Nakamura, T. Takeuchi, Y. Haga, E. Yamamoto, H. Harima, M. Hedo, T. Nakama and Y. Onuki, *J. Electron. Mater.* **46** (2017) 3572-3586.

## Noguchi group

We have studied the membrane shape transformations by proteins. (1) tubulation and rupture by the absorption of banana-shaped proteins. (2) high-genus stomatocyte (nuclear envelope shape) constructed by osmotic pressure and pore-size constraint by nuclear pore complex. We have also proposed new force decomposition methods of multibody potentials to calculate local stress and found that the obtained local stress largely depends on the decompositions even when they satisfy the conservation of translational and angular momentum.

1. Unveiling Dimensionality Dependence of Glassy Dynamics: 2D Infinite Fluctuation Eclipses Inherent Structural Relaxation: H. Shiba, Y. Yamada, T. Kawasaki and K. Kim, *Phys. Rev. Lett.* **117** (2016) 245701.
2. Nonuniqueness of local stress of three-body potentials in molecular simulations: K. M. Nakagawa and H. Noguchi, *Phys. Rev. E* **94** (2016) 053304(1-11).
3. Shape deformation of lipid membranes by banana-shaped protein rods: Comparison with isotropic inclusions and membrane rupture: H. Noguchi, *Phys. Rev. E* **93** (2016) 052404(1-10).
4. † Monte Carlo study of the frame, fluctuation and internal tensions of fluctuating membranes with fixed area: H. Shiba, H. Noguchi and J.-B. Fournier, *Soft Matter* **12** (2016) 2373-2380.
5. Membrane tubule formation by banana-shaped proteins with or without transient network structure: H. Noguchi, *Sci. Rep.* **6** (2016) 20935.
6. Rheological evaluation of colloidal dispersions using the smoothed profile method: formulation and applications: J. J. Molina, K. Otomura, H. Shiba, H. Kobayashi, M. Sano and R. Yamamoto, *J. Fluid Mech.* **792** (2016) 590-619.
7. Construction of Nuclear Envelope Shape by a High-Genus Vesicle with Pore-Size Constraint: H. Noguchi, *Biophys. J.* **111** (2016) 824-831.
8. 分子シミュレーションにおける三体ポテンシャルを含んだ系の局所応力テンソルの非一意性: 中川 恒, 分子シミュレーション研究会会誌 “アンサンプル” **19** (2017) 69.

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\* Joint research among groups within ISSP.

9. Membrane structure formation induced by two types of banana-shaped proteins: H. Noguchi/ and J.-B. Fournier, *Soft Matter* (2017), accepted for publication.

## Materials Synthesis and Characterization group

1. †\* Pressure-induced non-superconducting phase of  $\beta$ - $\text{Na}_{0.33}\text{V}_2\text{O}_5$  and the mechanism of high-pressure phase transitions in  $\beta$ - $\text{Na}_{0.33}\text{V}_2\text{O}_5$  and  $\beta$ - $\text{Li}_{0.33}\text{V}_2\text{O}_5$  at room temperature: A. Grzechnik, Y. Ueda, T. Yamauchi, M. Hanfland, P. Hering, V. Potapkin and K. Friese, *J. Phys.: Condens. Matter* **28** (2016) 035401(1-9).
2. †\* Hybrid Amine-Functionalized Graphene Oxide as a Robust Bifunctional Catalyst for Atmospheric Pressure Fixation of Carbon Dioxide using Cyclic Carbonates: V. B. Saptal, T. Sasaki, K. Harada, D. Nishio-Hamane and B. M. Bhanage, *ChemSusChem* **9** (2016) 644.
3. †\* Light and SEM observation of opal phytoliths in the mulberry leaf: O. Tsutsui, R. Sakamoto, M. Obayashi, S. Yamakawa, T. Handa, D. Nishio-Hamane and I. Matsuda, *Flora* **218** (2016) 44-50.
4. †\* Bunnoite, a new hydrous manganese aluminosilicate from Kamo Mountain, Kochi prefecture, Japan: D. Nishio-Hamane, K. Momma, R. Miyawaki and T. Minakawa, *Miner Petrol* **110** (2016) 917.
5. \* Weak ferromagnetic order breaking the threefold rotational symmetry of the underlying kagome lattice in  $\text{CdCu}_3(\text{OH})_6(\text{NO}_3)_2 \cdot \text{H}_2\text{O}$ : R. Okuma, T. Yajima, D. Nishio-Hamane, T. Okubo and Z. Hiroi, *Phys. Rev. B* **95** (2017) 094427.
6. \* Post-Cotunnite Phase Transition in Zirconia at High Pressure: D. Nishio-Hamane, in: *Photon Factory Highlights 2015* (KEK, 2016), 38-39.

## Neutron Science Laboratory

### Shibayama group

Shibayama group has been exploring the structure and dynamics of soft matter, especially polymer gels, micelles, thermo-responsive polymers, and thermosets, utilizing a combination of small-angle neutron scattering (SANS), small-angle X-ray scattering (SAXS), and dynamic light scattering (DLS). The objectives are to elucidate the relationship between the structure and variety of novel properties/functions of polymer gels/resins. The highlights of 2016 include investigation of (1) solvated structure of thermo-responsive polymers in ionic liquid, (2) structure of amphiphilic conetworks, (3) crosslinking inhomogeneities of phenolic resins, (4) pressure response of thermo-responsive polymer in ionic liquid, and (5) dynamic light scattering microscopy of turbid systems, (6) probe-SAXS of hydrogels under elongation, and so on.

1. Cross-link inhomogeneity in phenolic resins at the initial stage of curing studied by 1H-pulse NMR spectroscopy and complementary SAXS/WAXS and SANS/WANS with a solvent-swelling technique: A. Izumi, Y. Shudo, T. Nakao and M. Shibayama, *Polymer* **103** (2016) 152-162.
2. Large-scale molecular dynamics simulation of crosslinked phenolic resins using pseudo-reaction model: Y. Shudo, A. Izumi, K. Hagita, T. Nakao and M. Shibayama, *Polymer* **103** (2016) 261-276.
3. † Mechanism of heat-induced gelation for ovalbumin and its N-terminus cleaved form: T. Hiroi, Y. Okazumi, K. C. Littrell, Y. Narita, N. Tanaka and M. Shibayama, *Polymer* **93** (2016) 152-158.
4. † Fabrication and Structural Characterization of Module-Assembled Amphiphilic Conetwork Gels: T. Hiroi, S. Kondo, T. Sakai, E. P. Gilbert, Y.-S. Han, T.-H. Kim and M. Shibayama, *Macromolecules* **49** (2016) 4940-4947.
5. Nearly Ideal Polymer Network Ion Gel Prepared in pH-Buffering Ionic Liquid: K. Hashimoto, K. Fujii, K. Nishi, T. Sakai and M. Shibayama, *Macromolecules* **49** (2016) 344-352.
6. Pressure Response of a Thermo-responsive Polymer in an Ionic Liquid: K. Hirose, K. Fujii, T. Ueki, Y. Kitazawa, M. Watanabe and M. Shibayama, *Macromolecules* **49** (2016) 8249-8253.
7. Transitions of Aggregation States for Concentrated Carbon Nanotube Dispersion: T. Hiroi, S. Ata and M. Shibayama, *J. Phys. Chem. C* **120** (2016) 5776-5782.
8. SANS study on the solvated structure and molecular interactions of a thermo-responsive polymer in a room temperature ionic liquid: K. Hirose, K. Fujii, T. Ueki, Y. Kitazawa, K. C. Littrell, M. Watanabe and M. Shibayama, *Phys. Chem. Chem. Phys.* **18** (2016) 17881-17889.

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† Joint research with outside partners.

9. Probe-SAXS on hydrogels under elongation: K. Nishi and M. Shibayama, *Soft Matter* **12** (2016) 5334-5339.
10. Structural Study on Aggregation Behavior of Star-Type Trimeric Surfactants in the Presence of Organic Salts: T. Kusano, K. Akutsu, H. Iwase, T. Yoshimura and M. Shibayama, *Colloids & Surfaces A* **497** (2016) 109-116.
11. Structure-mechanical property relationships in crosslinked phenolic resin investigated by molecular dynamics simulation: Y. Shudo, A. Izumi, K. Hagita, T. Nakao and M. Shibayama, *Polymer* **116** (2017) 506-514.
12. Decisive test of the ideal behavior of tetra-PEG gels: F. Horkay, K. Nishi and M. Shibayama, *J. Chem. Phys.* **146** (2017) 164905(1-8).
13. <sup>†</sup>Microscopic Structure of the “Nonswellable” Thermoresponsive Amphiphilic Conetwork: S. Nakagawa, X. Li, H. Kamata, T. Sakai, E. P. Gilbert and M. Shibayama, *Macromolecules* **50** (2017) 3388.
14. Probe Diffusion of Sol–Gel Transition in an Isorefractive Polymer Solution: X. Li, N. Watanabe, T. Sakai and M. Shibayama, *Macromolecules* **50** (2017) 2916.
15. Exploration of Ideal Polymer Networks: M. Shibayama, *Macromol. Symp* **372** (2017) 7-13.
16. Effect of protonation on the solvation structure of solute N-butylamine in an aprotic ionic liquid: K. Hashimoto, K. Fujii, K. Ohara and M. Shibayama, *Phys. Chem. Chem. Phys.* **19** (2017) 8194-8200.
17. Measurement of Particle Size Distribution in Turbid Solutions by Dynamic Light Scattering Microscopy: T. Hiroi and M. Shibayama, *JoVE* **119** (2017) 54885.
18. Fast-forming hydrogel with ultralow polymeric content as an artificial vitreous body: K. Hayashi, F. Okamoto, S. Hoshi, T. Katashima, D. C. Zujur, X. Li, M. Shibayama, E. P. Gilbert, U.-I. Chung, S. Ohba, T. Oshika and T. Sakai, *Nat. Biomed. Eng.* **1** (2017) 0044(1-7).
19. Small-angle Neutron Scattering of Polysaccharide Hydrogels: M. Shibayama, in: *Polysaccharide hydrogels: Characterization and Biomedical Applications*, Ch 7, edited by Matricardi, P; Alhaique, F; Coviello, T., (Pan Stanford Publishing Pte. Ltd., Singapore, 2016), 245-264.

### Yoshizawa group

A systematic study on a family of Ce-based non-centrosymmetric heavy fermion compounds CeTSi<sub>3</sub> (T=transition metal ions) were studied, and the M-T phase diagram was established for CePdSi<sub>3</sub>. It is found that CePdSi<sub>3</sub> shows extremely complicated multi-metamagnetic transitions. In order to elucidate such complicated magnetic phase diagram and magnetic properties from a microscopic basis, the crystalline electric field levels were studied for T=Pd, Pt, and Rh compounds with use of inelastic neutron scattering measurements.

1. Inelastic Neutron Scattering Study of Stripe and Overdoped Checkerboard Ordering in Layered Nickel Oxide d<sub>2-x</sub>Sr<sub>x</sub>NiO<sub>4</sub>: Y. Ikeda, S. Suzuki, T. Nakabayashi, H. Yoshizawa, T. Yokoo and S. Itoh, *J. Phys. Soc. Jpn.* **85** (2016) 023701.
2. <sup>†\*</sup>Superconductivity and Non-Fermi-Liquid Behavior in the Heavy-Fermion Compound CeCo<sub>1-x</sub>Ni<sub>x</sub>In<sub>5</sub>: R. Otaka, M. Yokoyama, H. Mashiko, T. Hasegawa, Y. Shimizu, Y. Ikeda, K. Tenya, S. Nakamura, D. Ueta, H. Yoshizawa and T. Sakakibara, *J. Phys. Soc. Jpn.* **85** (2016) 094713.
3. Weak Ferromagnetism and Multiple Metamagnetic Transitions in the Non-centrosymmetric Tetragonal Compound CePdSi<sub>3</sub>: D. Ueta, Y. Ikeda and H. Yoshizawa, *J. Phys. Soc. Jpn.* **85** (2016) 104703.

### Yamamuro group

Our laboratory is studying chemical physics of complex condensed matters by using neutron scattering, X-ray diffraction, calorimetric, dielectric, and viscoelastic techniques. Our target materials are glasses, liquids, and various disordered systems. This year, we have succeeded to measure synchrotron X-ray diffraction of glassy carbon disulfide (CS<sub>2</sub>), propane (CH<sub>3</sub>CH<sub>2</sub>CH<sub>3</sub>) and propene (CH<sub>3</sub>CHCH<sub>2</sub>). These glasses were prepared by vapor-deposition at 3 K by using a cryostat developed for in-situ X-ray diffraction experiments in SPring-8. It was found that the local structures of these simple molecular glasses are similar to those of their crystalline states. Another topic is that we found unusual glass transitions in liquid alkylated tetraphenylporphyrins (3,5-C<sub>6</sub>C<sub>10</sub>-TPP and 2,5-C<sub>6</sub>C<sub>10</sub>-TPP); they appeared in a wide temperature range between 150 and 230 K. It is amazing that these large molecules (molecular mass: 2538) exist in liquid states at room temperature. We named these liquids “super-high entropy liquids”. Other than above topics, we have obtained neutron diffraction data of nanoparticles of PdPtD and PdRuD alloy hydride systems. The analysis is going on.

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\* Joint research among groups within ISSP.

1. X-ray Diffraction Study on Simple Molecular Glasses Created by Low-Temperature Vapor Deposition: Y. Mizuno, M. Kofu and O. Yamamuro, *J. Phys. Soc. Jpn.* **85** (2016) 124602.
2. Hydrogen diffusion in bulk and nanocrystalline palladium: A quasielastic neutron scattering study: M. Kofu, N. Hashimoto, H. Akiba, H. Kobayashi, H. Kitagawa, M. Tyagi, A. Faraone, J. R. D. Copley, W. Lohstroh and O. Yamamuro, *Phys. Rev. B* **94** (2016) 064303.
3. Nanometer-Size Effect on Hydrogen Sites in Palladium Lattice: H. Akiba, M. Kofu, H. Kobayashi, H. Kitagawa, K. Ikeda, T. Otomo and O. Yamamuro, *J. Am. Chem. Soc.* **138** (2016) 10238.
4. Connecting thermodynamics and dynamics in a supercooled liquid: Cresolphthalein-dimethylether: S. Samanta, O. Yamamuro and R. Richert, *Thermochimica Acta* **636** (2016) 57-62.
5. Effect of water on the structure of a prototype ionic liquid: O. Borodin, D. L. Price, B. Aoun, M. A. González, J. B. Hooper, M. Kofu, S. Kohara, O. Yamamuro and M.-L. Saboungi, *Phys. Chem. Chem. Phys.* **18** (2016) 23474.
6. †Relaxation in a Prototype Ionic Liquid: Influence of Water on the Dynamics: D. L. Price, O. Borodin, M. A. González, M. Kofu, K. Shibata, T. Yamada, O. Yamamuro and M.-L. Saboungi, *J. Phys. Chem. Lett.* **8** (2017) 715.
7. Calorimetric and Neutron Scattering Studies on Glass Transitions and Ionic Diffusions in Imidazolium-based Ionic Liquids: O. Yamamuro and M. Kofu, *IOP Conference Series: Materials Science and Engineering* (2017), accepted for publication.
8. 低温蒸着法で作製した単純分子ガラスの構造: 山室 修, 水野 勇希, 古府 麻衣子, *日本結晶学会誌* **58** (2016) 13-17.
9. イミダゾリウム系イオン液体の階層的・ガラスダイナミクス: 古府 麻衣子, 山室 修, *日本結晶学会誌* **58** (2016) 18-23.
10. 熱測定と中性子散乱の相補利用による新規物質研究: 山室 修, 熱測定 (2017), accepted for publication.
11. イオン液体の熱的挙動, ダイナミクス: 山室 修, 古府 麻衣子, 「イオン液体研究最前線と社会実装」, 2, 渡邊 正義, (シーエムシー出版, 2016), 13-24.
12. ガラス転移温度: 山室 修, 「化学便覧基礎編改訂第6版」, 10.15, 日本化学会編, (丸善出版, 2017), accepted for publication.

## Masuda group

The goal of our research is to discover a new quantum phenomenon and to reveal the mechanism of it. In this fiscal year we studied the following topics; magnetic order in a buckled honeycomb lattice antiferromagnet, spin model of O<sub>2</sub>-based magnet in a nanoporous metal complex, dielectric and magnetic properties in relaxor magnet, magnetic excitations in a quantum breathing pyrochlore antiferromagnet, and continuous control of local magnetic moment by applied electric field in a multiferroic material.

1. Crystal Field Excitations in the Breathing Pyrochlore Antiferromagnet Ba<sub>3</sub>Yb<sub>2</sub>Zn<sub>5</sub>O<sub>11</sub>: T. Haku, M. Soda, M. Sera, K. Kimura, S. Itoh, T. Yokoo and T. Masuda, *J. Phys. Soc. Jpn.* **85** (2016) 034721.
2. Dielectric and Magnetic Properties in Relaxor Magnet LuFeCoO<sub>4</sub>: M. Soda and T. Masuda, *J. Phys. Soc. Jpn.* **85** (2016) 034713.
3. Spin Model of O<sub>2</sub>-Based Magnet in a Nanoporous Metal Complex: M. Soda, Y. Honma, S. Takamizawa, S. Ohira-Kawamura, K. Nakajima and T. Masuda, *J. Phys. Soc. Jpn.* **85** (2016) 034717.
4. Continuous control of local magnetic moment by applied electric field in multiferroics Ba<sub>2</sub>CoGe<sub>2</sub>O<sub>7</sub>: M. Soda, S. Hayashida, B. Roessli, M. Månsson, J. S. White, M. Matsumoto, R. Shiina and T. Masuda, *Phys. Rev. B* **94** (2016) 094418.
5. Low-energy excitations and ground-state selection in the quantum breathing pyrochlore antiferromagnet Ba<sub>3</sub>Yb<sub>2</sub>Zn<sub>5</sub>O<sub>11</sub>: T. Haku, K. Kimura, Y. Matsumoto, M. Soda, M. Sera, D. Yu, R. A. Mole, T. Takeuchi, S. Nakatsuji, Y. Kono, T. Sakakibara, L. -J. Chang and T. Masuda, *Phys. Rev. B* **93** (2016) 220407.
6. Magnetic ordering of the buckled honeycomb lattice antiferromagnet Ba<sub>2</sub>NiTeO<sub>6</sub>: S. Asai, M. Soda, K. Kasatani, T. Ono, M. Avdeev and T. Masuda, *Phys. Rev. B* **93** (2016) 024412.
7. Crystal field excitations on NdFe<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> investigated by inelastic neutron scattering: S. Hayashida, M. Soda, S. Itoh, T. Yokoo, K. Ohgushi, D. Kawana and T. Masuda, *J. Phys.: Conf. Ser.* **746** (2016) 012059.

† Joint research with outside partners.

8. Magnetic Structure and Dielectric State in the Multiferroic  $\text{Ca}_2\text{CoSi}_2\text{O}_7$ : M. Soda, S. Hayashida, T. Yoshida, M. Akaki, M. Hagiwara, M. Avdeev, O. Zaharko and T. Masuda, *J. Phys. Soc. Jpn.* **86** (2017) 064703(1-5).
9. Spin pseudogap in the  $S=1/2$  chain material  $\text{Sr}_2\text{CuO}_3$  with impurities: G. Simutis, S. Gvasaliya, N. S. Beesetty, T. Yoshida, J. Robert, S. Petit, A. I. Kolesnikov, M. B. Stone, F. Bourdarot, H. C. Walker, D. T. Adroja, O. Sobolev, C. Hess, T. Masuda, A. Revcolevschi, B. Büchner and A. Zheludev, *Phys. Rev. B* **95** (2017) 054409.
10. A layered wide-gap oxyhalide semiconductor with an infinite  $\text{ZnO}_2$  square planar sheet:  $\text{Sr}_2\text{ZnO}_2\text{Cl}_2$ : Y. Su, Y. Tsujimoto, A. Miura, S. Asai, M. Avdeev, H. Ogino, M. Ako, A. A. Belik, T. Masuda, T. Uchikoshi and K. Yamaura, *Chem. Commun.* **53** (2017) 3826-3829.
11. Dielectric Property and Diffuse Scattering in Relaxor Magnet  $\text{LuFeCoO}_4$ : M. Soda and T. Masuda, *J. Phys.: Conf. Ser.* **828** (2017) 012001.
12. Neutron Scattering Study in Breathing Pyrochlore Antiferromagnet  $\text{Ba}_3\text{Yb}_2\text{Zn}_5\text{O}_{11}$ : T. Haku, M. Soda, M. Sera, K. Kimura, J. Taylor, S. Itoh, T. Yokoo, Y. Matsumoto, D. Yu, R. A. Mole, T. Takeuchi, S. Nakatsuji, Y. Kono, T. Sakakibara, L. -J. Chang and T. Masuda, *J. Phys.: Conf. Ser.* **828** (2017) 012018.
13. Powder neutron diffraction in one-dimensional frustrated chain compound  $\text{NaCuMoO}_4(\text{OD})$ : S. Asai, T. Oyama, M. Soda, K. Rule, K. Nawa, Z. Hiroi and T. Masuda, *J. Phys.: Conf. Ser.* **828** (2017) 012006.
14. Hyperthermia and chemotherapy using Fe(Salen) nanoparticles might impact glioblastoma treatment: M. Ohtake, M. Umemura, I. Sato, T. Akimoto, K. Oda, A. Nagasako, J.-H. Kim, T. Fujita, U. Yokoyama, T. Nakayama, Y. Hoshino, M. Ishiba, S. Tokura, M. Hara, T. Muramoto, S. Yamada, T. Masuda, I. Aoki, Y. Takemura, H. Murata, H. Eguchi, N. Kawahara and Y. Ishikawa, *Sci. Rep.* **7** (2017) 42783.
15. Magnetic metal-complex-conducting copolymer core-shell nanoassemblies for a single-drug anticancer platform: J.-H. Kim, H. Eguchi, M. Umemura, I. Sato, S. Yamada, Y. Hoshino, T. Masuda, I. Aoki, K. Sakurai, M. Yamamoto and Y. Ishikawa, *NPG Asia Mater* **9** (2017) e367.

## International MegaGauss Science Laboratory

### Takeyama group

1000 T class electro-magnetic flux compression megagauss generators were reconstructed and completed. A peak magnetic field of 450 T is obtained by the megagauss generator with less than 1 MJ energy injection. Magnetization measurement techniques are still in progress in the single-turn coil megagauss generator system, and the measurements using a co-axial type self-compensated pick-up-coil up to 130 T, and using magneto-optical techniques up to 200 T are currently achieved with high reliability, at very low temperature around 5 K. The methods have been applied to investigate spin structures of frustrated magnetic materials, multi-ferro materials, and quantum spin systems, etc.

1. †Irreversible Heating Measurement with Microsecond Pulse Magnet: Example of the  $\alpha$ - $\theta$  Phase Transition of Solid Oxygen: T. Nomura, Y. H. Matsuda, S. Takeyama and T. C. Kobayashi, *J. Phys. Soc. Jpn.* **85** (2016) 094601(1-5).
2. †\*Electric Polarization Induced by Spin Ordering under Magnetic Fields in Distorted Triangular Lattice Antiferromagnet  $\text{RbCoBr}_3$ : Y. Nishiwaki, M. Tokunaga, R. Sakakura, S. Takeyama, T. Kato and K. Iio, *J. Phys. Soc. Jpn.* **86** (2017) 044701(1-7).
3. \*Magnetic transitions under ultrahigh magnetic fields of up to 130 T in the breathing pyrochlore antiferromagnet  $\text{LiInCr}_4\text{O}_8$ : Y. Okamoto, D. Nakamura, A. Miyake, S. Takeyama, M. Tokunaga, A. Matsuo, K. Kindo and Z. Hiroi, *Phys. Rev. B* **95** (2017) 134438.
4. Excitation energy dependence of initial phase shift in Kerr rotation of resident electron spin polarization in a CdTe single quantum well: L. -P. Yan, T. Takamura, R. Kaji, G. Karczewski, S. Takeyama and S. Adachi, *Phys. Status Solidi B* **254** (2017) 1600449(1-6).

### Kindo group

The specific heat measurements under long pulsed magnetic field up to 43.5 T has been open for the joint-use research. Repetition of the maximum field generation is limited to three times in a day due to a cooling time for the magnet. We are making new high repetitive magnet to carry out the measurements at higher frequency.

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\* Joint research among groups within ISSP.

1. †Evidence of Charge Transfer and Orbital Magnetic Moment in Multiferroic CuFeO<sub>2</sub>: Y. Narumi, T. Nakamura, H. Ikeno, N. Terada, T. Morioka, K. Saito, H. Kitazawa, K. Kindo and H. Nojiri, *J. Phys. Soc. Jpn.* **85** (2016) 114705.
2. †Large Magnetoresistance and Volume Expansion Associated with Valence Transition in Eu(Rh<sub>1-x</sub>Ir<sub>x</sub>)<sub>2</sub>Si<sub>2</sub>: A. Mitsuda, T. Fujimoto, E. Kishaba, S. Hamano, A. Kondo, K. Kindo and H. Wada, *J. Phys. Soc. Jpn.* **85** (2016) 124703.
3. †\*Magnetic and Structural Studies on Two-Dimensional Antiferromagnets (MCl)LaNb<sub>2</sub>O<sub>7</sub> (M = Mn, Co, Cr): A. Kitada, Y. Tsujimoto, M. Nishi, A. Matsuo, K. Kindo, Y. Ueda, Y. Ajiro and H. Kageyama, *J. Phys. Soc. Jpn.* **85** (2016) 034005(6).
4. †\*Valence State in CeIrIn<sub>5</sub> at High Magnetic Fields of up to 42 T: Y. H. Matsuda, T. T. Terashima, K. Kindo, R. Tsunoda, R. Settai, N. Kawamura, M. Mizumaki and T. Inami, *J. Phys. Soc. Jpn.* **85** (2016) 115001(1-2).
5. †Field-driven successive phase transitions in the quasi-two-dimensional frustrated antiferromagnet Ba<sub>2</sub>CoTeO<sub>6</sub> and highly degenerate classical ground states: P. Chanlert, N. Kurita, H. Tanaka, D. Goto, A. Matsuo and K. Kindo, *Phys. Rev. B* **93** (2016) 094420(7).
6. †Magnetism of the antiferromagnetic spin-1/2 tetramer compound CuInVO<sub>5</sub>: M. Hase, M. Matsumoto, A. Matsuo and K. Kindo, *Phys. Rev. B* **94** (2016) 174421.
7. †Origin of positive out-of-plane magnetoconductivity in overdoped Bi<sub>1.6</sub>Pb<sub>0.4</sub>Sr<sub>2</sub>CaCu<sub>1.96</sub>Fe<sub>0.04</sub>O<sub>8+δ</sub>: T. Watanabe, T. Usui, S. Adachi, Y. Teramoto, M. M. Dobroka, I. Kakeya, A. Kondo, K. Kindo and S. Kimura, *Phys. Rev. B* **94** (2016) 174517.
8. †\*Quasi-two-dimensional Bose-Einstein condensation of spin triplets in the dimerized quantum magnet Ba<sub>2</sub>CuSi<sub>2</sub>O<sub>6</sub>Cl<sub>2</sub>: M. Okada, H. Tanaka, N. Kurita, K. Johmoto, H. Uekusa, A. Miyake, M. Tokunaga, S. Nishimoto, M. Nakamura, M. Jaime, G. Radtke and A. Saúl, *Phys. Rev. B* **94** (2016) 094421(1-8).
9. †\*Spin state ordering of strongly correlating LaCoO<sub>3</sub> induced at ultrahigh magnetic fields: A. Ikeda, T. Nomura, Y. H. Matsuda, A. Matsuo, K. Kindo and K. Sato, *Phys. Rev. B* **93** (2016) 220401(1-5).
10. †Various disordered ground states and 1/3 magnetization-plateau-like behavior in the S=1/2 Ti<sup>3+</sup> kagome lattice antiferromagnets Rb<sub>2</sub>NaTi<sub>3</sub>F<sub>12</sub>, Cs<sub>2</sub>NaTi<sub>3</sub>F<sub>12</sub>, and Cs<sub>2</sub>KTi<sub>3</sub>F<sub>12</sub>: M. Goto, H. Ueda, C. Michioka, A. Matsuo, K. Kindo and K. Yoshimura, *Phys. Rev. B* **94** (2016) 104432.
11. †90 K superconductivity of clean Pb1212 epitaxial films: S. Komori, A. Kondo, K. Kindo and I. Kakeya, *Supercond. Sci. Technol.* **29** (2016) 085007.
12. \*Experimental exploration of novel semimetal state in strong anisotropic Pyrochlore iridate Nd<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub> under high magnetic field: Z. M. Tian, Y. Kohama, T. Tomita, J. Ishikawa, H. Mairo, K. Kindo and S. Nakatsuji, *J. Phys.: Conf. Ser.* **683** (2016) 012024(6).
13. \*Frustrated magnetism in a Mott insulator based on a transition metal chalcogenide: S. Kawamoto, T. Higo, T. Tomita, S. Suzuki, Z. M. Tian, K. Mochizuki, A. Matsuo, K. Kindo and S. Nakatsuji, *J. Phys.: Conf. Ser.* **683** (2016) 012025(4).
14. Repeating pulsed magnet system for axion-like particle searches and vacuum birefringence experiments: T. Yamazaki, T. Inada, T. Namba, S. Asai, T. Kobayashi, A. Matsuo, K. Kindo and H. Nojiri, *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* **833** (2016) 122.
15. †Fe Substitution Effect on the High-Field Magnetization in the Kondo Semiconductor CeRu<sub>2</sub>Al<sub>10</sub>: A. Kondo, K. Kindo, H. Nohara, M. Nakamura, H. Tanida, M. Sera and T. Nishioka, *J. Phys. Soc. Jpn.* **86** (2017) 023705.
16. †\*Magnetization Process of the Kondo Insulator YbB<sub>12</sub> in Ultrahigh Magnetic Fields: T. T. Terashima, A. Ikeda, Y. H. Matsuda, A. Kondo, K. Kindo and F. Iga, *J. Phys. Soc. Jpn.* **86** (2017) 054710(1-5).
17. \*Thermodynamic Investigation of Metamagnetic Transitions and Partial Disorder in the Quasi-Kagome Kondo Lattice CePdAl: K. Mochizuki, Y. Shimizu, A. Kondo, S. Nakamura, S. Kittaka, Y. Kono, T. Sakakibara, Y. Ikeda, Y. Isikawa and K. Kindo, *J. Phys. Soc. Jpn.* **86** (2017) 034709(1-5).
18. †\*α-β and β-γ phase boundaries of solid oxygen observed by adiabatic magnetocaloric effect: T. Nomura, Y. Kohama, Y. H. Matsuda, K. Kindo and T. C. Kobayashi, *Phys. Rev. B* **95** (2017) 104420.
19. High-field magnetization of Heusler compound Fe<sub>2</sub>Mn<sub>1-x</sub>V<sub>x</sub>Si: M. Hiroi, T. Tazoko, H. Sano, I. Shigeta, K. Koyama, A. Kondo, K. Kindo, H. Manaka and N. Terada, *Phys. Rev. B* **95** (2017) 014410.
20. \*Magnetic transitions under ultrahigh magnetic fields of up to 130 T in the breathing pyrochlore antiferromagnet LiInCr<sub>4</sub>O<sub>8</sub>: Y. Okamoto, D. Nakamura, A. Miyake, S. Takeyama, M. Tokunaga, A. Matsuo, K. Kindo and Z. Hiroi, *Phys. Rev. B* **95** (2017) 134438.

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† Joint research with outside partners.

21. †\*Magnetoelectric Behavior from S=1/2 Asymmetric Square Cupolas: Y. Kato, K. Kimura, A. Miyake, M. Tokunaga, A. Matsuo, K. Kindo, M. Akaki, M. Hagiwara, M. Sera, T. Kimura and Y. Motome, *Phys. Rev. Lett.* **118** (2017) 107601 (1-5).
22. Search for Two-Photon Interaction with Axionlike Particles Using High-Repetition Pulsed Magnets and Synchrotron X Rays: T. Inada, T. Yamazaki, T. Namba, S. Asai, T. Kobayashi, K. Tamasaku, Y. Tanaka, Y. Inubushi, K. Sawada, M. Yabashi, T. Ishikawa, A. Matsuo, K. Kawaguchi, K. Kindo and H. Nojiri, *Phys. Rev. Lett.* **118** (2017) 071803.
23. \*Giant Exchange Coupling Evidenced with a Magnetization Jump at 52 T for a Gadolinium-Nitroxide Chelate: T. Kanetomo, T. Kihara, A. Miyake, A. Matsuo, M. Tokunaga, K. Kindo, H. Nojiri and T. Ishida, *Inorg. Chem.* **56** (2017) 3310-3314.
24. Magnetic and electrical properties of Heusler compounds  $Ru_2Cr_{1-x}X_xSi$  (X = V, Ti): M. Hiroi, H. Sano, T. Tazoko, I. Shigeta, M. Ito, K. Koyama, H. Manaka, N. Terada, M. Fujii, A. Kondo and K. Kindo, *J. Alloys Compd.* **694** (2017) 1376.
25. \*パイロクロア型イリジウム酸化物  $Nd_2Ir_2O_7$  における磁場印加方向に敏感な金属-絶縁体転移: 小濱 芳允, Z. Tian, 富田 崇弘, 石川 洵, 金道 浩一, 石塚 大晃, 中辻 知, *固体物理* **51** (2016) 339-355.

## Tokunaga group

Multiferroic materials have been extensively studied partly because of their possible application to the memory devices with low power consumption. Our careful experiments revealed non-volatile magnetoelectric memory effects in a well-known multiferroic material,  $BiFeO_3$ . We found application of positive (negative) electric fields to a sample causes decrease (increase) in the resistance. This bipolar RRAM effect observed at room temperature will be useful for memory devices.

1. †Spin Structure Change in Co-Substituted  $BiFeO_3$ : H. Yamamoto, T. Kihara, K. Oka, M. Tokunaga, K. Mibu and M. Azuma, *J. Phys. Soc. Jpn.* **85** (2016) 064704(1-4).
2. †\*Magnetic-field-induced spin crossover of Y-doped  $Pr_{0.7}Ca_{0.3}CoO_3$ : A. Ikeda, S. Lee, T. T. Terashima, Y. H. Matsuda, M. Tokunaga and T. Naito, *Phys. Rev. B* **94** (2016) 115129(1-8).
3. †\*Quasi-two-dimensional Bose-Einstein condensation of spin triplets in the dimerized quantum magnet  $Ba_2CuSi_2O_6Cl_2$ : M. Okada, H. Tanaka, N. Kurita, K. Johmoto, H. Uekusa, A. Miyake, M. Tokunaga, S. Nishimoto, M. Nakamura, M. Jaime, G. Radtke and A. Saúl, *Phys. Rev. B* **94** (2016) 094421(1-8).
4. 圧力下の半金属黒燐における異常量子輸送現象: 秋葉 和人, 三宅 厚志, 徳永 将史, 赤浜 裕一, *固体物理* **51** (2016) 249.
5. Resistive memory effects in  $BiFeO_3$  single crystals controlled by transverse electric fields: S. Kawachi, H. Kuroe, T. Ito, A. Miyake and M. Tokunaga, *Appl. Phys. Lett.* **108** (2016) 162903(1-4).
6. †Quantum Hall effect in a bulk antiferromagnet  $EuMnBi_2$  with magnetically confined two-dimensional Dirac fermions: H. Masuda, H. Sakai, M. Tokunaga, Y. Yamasaki, A. Miyake, J. Shiogai, S. Nakamura, S. Awaji, A. Tsukazaki, H. Nakao, Y. Murakami, T. -h. Arima, Y. Tokura and S. Ishiwata, *Science Advances* **2** (2016) e1501117(1-6).
7. †\*Electric Polarization Induced by Spin Ordering under Magnetic Fields in Distorted Triangular Lattice Antiferromagnet  $RbCoBr_3$ : Y. Nishiwaki, M. Tokunaga, R. Sakakura, S. Takeyama, T. Kato and K. Iio, *J. Phys. Soc. Jpn.* **86** (2017) 044701(1-7).
8. \*Magnetic transitions under ultrahigh magnetic fields of up to 130 T in the breathing pyrochlore antiferromagnet  $LiInCr_4O_8$ : Y. Okamoto, D. Nakamura, A. Miyake, S. Takeyama, M. Tokunaga, A. Matsuo, K. Kindo and Z. Hiroi, *Phys. Rev. B* **95** (2017) 134438.
9. \*Two-carrier analyses of the transport properties of black phosphorus under pressure: K. Akiba, A. Miyake, Y. Akahama, K. Matsubayashi, Y. Uwatoko and M. Tokunaga, *Phys. Rev. B* **95** (2017) 115126(1-7).
10. †\*Magnetoelectric Behavior from S=1/2 Asymmetric Square Cupolas: Y. Kato, K. Kimura, A. Miyake, M. Tokunaga, A. Matsuo, K. Kindo, M. Akaki, M. Hagiwara, M. Sera, T. Kimura and Y. Motome, *Phys. Rev. Lett.* **118** (2017) 107601(1-5).
11. \*Giant Exchange Coupling Evidenced with a Magnetization Jump at 52 T for a Gadolinium-Nitroxide Chelate: T. Kanetomo, T. Kihara, A. Miyake, A. Matsuo, M. Tokunaga, K. Kindo, H. Nojiri and T. Ishida, *Inorg. Chem.* **56** (2017) 3310-3314.

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\* Joint research among groups within ISSP.

## Y. Matsuda group

Spin state degree of freedom of cobalt oxides has been attracting much attention of scientists for a long time. The electronic and structural properties as well as the magnetic properties sometimes change dramatically. LaCoO<sub>3</sub> is one of the canonical cobalt oxides and has been studied for more than half century owing to its peculiar properties. We have investigated the magnetization process of LaCoO<sub>3</sub> in high magnetic fields of up to 133 T at several temperatures. In addition to the previously known magnetization jump at around 65 T at low temperatures, a novel phase has been observed to appear in higher fields when temperature is higher than about 30 K. The phase boundary in field-temperature (B-T) plane indicates this phase has lower entropy than the low field phase. The transition field increases with temperature and becomes higher than 130 T at 105 K. The spatial ordered state of the different spin states, namely high spin (S=2), intermediate spin (S=1) and low spin (S=0) states, is suggested. From theoretical point of view, field-induced transition to an excitonic insulating state possibly explains the observed phenomenon. Another cobalt oxide (Pr<sub>1-x</sub>Y<sub>x</sub>)<sub>0.7</sub>Ca<sub>0.3</sub>CoO<sub>3</sub> has also been studied in ultrahigh fields of up to 140 T and found that the B-T phase diagram determined by the magnetization and electric resistivity is qualitatively different from that of LaCoO<sub>3</sub>. We also studied the magnetic field induced phase transition of solid oxygen using irreversible heating effect. In SPring-8, using a pulsed magnet being combined with intense synchrotron x-rays, the valence state of Ce in the heavy fermion compound CeIrIn<sub>5</sub> was directly examined in high magnetic fields of up to 40 T at 2 K.

1. † Irreversible Heating Measurement with Microsecond Pulse Magnet: Example of the  $\alpha$ - $\theta$  Phase Transition of Solid Oxygen: T. Nomura, Y. H. Matsuda, S. Takeyama and T. C. Kobayashi, *J. Phys. Soc. Jpn.* **85** (2016) 094601(1-5).
2. †\* Valence State in CeIrIn<sub>5</sub> at High Magnetic Fields of up to 42 T: Y. H. Matsuda, T. T. Terashima, K. Kindo, R. Tsunoda, R. Settai, N. Kawamura, M. Mizumaki and T. Inami, *J. Phys. Soc. Jpn.* **85** (2016) 115001(1-2).
3. †\* Magnetic-field-induced spin crossover of Y-doped Pr<sub>0.7</sub>Ca<sub>0.3</sub>CoO<sub>3</sub>: A. Ikeda, S. Lee, T. T. Terashima, Y. H. Matsuda, M. Tokunaga and T. Naito, *Phys. Rev. B* **94** (2016) 115129(1-8).
4. †\* Spin state ordering of strongly correlating LaCoO<sub>3</sub> induced at ultrahigh magnetic fields: A. Ikeda, T. Nomura, Y. H. Matsuda, A. Matsuo, K. Kindo and K. Sato, *Phys. Rev. B* **93** (2016) 220401(1-5).
5. †\* Lifetime-Broadening-Suppressed X-ray Absorption Spectrum of  $\beta$ -YbAlB<sub>4</sub> Deduced from Yb 3d  $\rightarrow$  2p Resonant X-ray Emission Spectroscopy: N. Kawamura, N. Kanai, H. Hayashi, Y. H. Matsuda, M. Mizumaki, K. Kuga, S. Nakatsuji and S. Watanabe, *J. Phys. Soc. Jpn.* **86** (2017) 014711(1-7).
6. †\* Magnetization Process of the Kondo Insulator YbB<sub>12</sub> in Ultrahigh Magnetic Fields: T. T. Terashima, A. Ikeda, Y. H. Matsuda, A. Kondo, K. Kindo and F. Iga, *J. Phys. Soc. Jpn.* **86** (2017) 054710(1-5).
7. †\*  $\alpha$ - $\beta$  and  $\beta$ - $\gamma$  phase boundaries of solid oxygen observed by adiabatic magnetocaloric effect: T. Nomura, Y. Kohama, Y. H. Matsuda, K. Kindo and T. C. Kobayashi, *Phys. Rev. B* **95** (2017) 104420.

## Center of Computational Materials Science

### Akai group

(1) A scheme that combines the nonequilibrium Green's function method with the Korringa-Kohn-Rostoker Green's function method is proposed. The method is applied to Schottky junctions composed of an Al/GaN/Al trilayer. The results show that a Schottky barrier is formed at an undoped GaN and Al interface. The transport property of this system under various finite bias voltages is calculated. It is shown that the asymmetric behavior of electron transport against the direction of bias voltage occurs in this system, confirming the feature of rectification. (2) A classical spin model derived ab initio for rare-earth-based permanent magnet compounds is presented. Our target compound, NdFe12N, is a material that goes beyond today's champion magnet compound Nd<sub>2</sub>Fe<sub>14</sub>B in its intrinsic magnetic properties with a simpler crystal structure. Calculated temperature dependence of the magnetization and the anisotropy field agrees with the latest experimental results in the leading order. Having put the realistic observables under our numerical control, we propose that engineering 5d-electron-mediated indirect exchange coupling between 4f-electrons in Nd and 3d-electrons from Fe would most critically help enhance the material's utility over the operation-temperature range. (3) As a collaboration with experimental group, we have developed the method to calculate resonant MOKEZ spectra and apply it to the recent experiments performed at SPring8 by Kubota, et al. The ab-initio calculations explain the experimental results successfully, opening up the possibility to further extend the method so as to cover other systems such as compounds, disordered alloys and also to apply the second-harmonic generation.

1. Schottky junctions studied using Korringa-Kohn-Rostoker non-equilibrium Green's function method: M. Ogura and H. Akai, *J. Phys.: Condens. Matter* **85** (2016) 104715(1-7).

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† Joint research with outside partners.



2. Relevance of  $4f$ - $3d$  exchange to finite-temperature magnetism of rare-earth permanent magnets: An *ab-initio*-based spin model approach for  $\text{NdFe}_{12}\text{N}$ : M. Matsumoto, H. Akai, Y. Harashima, S. Doi and T. Miyake, *J. Appl. Phys.* **119** (2016) 213901(1-7).
3. Monte Carlo analysis for finite-temperature magnetism of  $\text{Nd}_2\text{Fe}_{14}\text{B}$  permanent magnet: Y. Toga, M. Matsumoto, S. Miyashita, H. Akai, S. Doi, T. Miyake and A. Sakuma, *Phys. Rev. B* **94** (2016) 174433(1-9).
4. Electrical resistivity of substitutionally disordered hcp Fe–Si and Fe–Ni alloys: Chemically-induced resistivity saturation in the Earth's core: H. Gomi, K. Hirose, H. Akai and Y. Fei, *Earth Planet. Sci. Lett.* **451** (2016) 51-61.
5. Atomistic-model study of temperature-dependent domain walls in the neodymium permanent magnet  $\text{Nd}_2\text{Fe}_{14}\text{B}$ : M. Nishino, Y. Toga, S. Miyashita, H. Akai, A. Sakuma and S. Hirose, *Phys. Rev. B* **95** (2017) 094429(1-7).
6. 磁石の秘密：赤井 久純，日本物理学会誌 **71** (2016) 277-281.

## Ozaki group

The X-ray photoelectron spectroscopy (XPS) has become one of the most important and widely used techniques in studying chemical composition and electronic states in the vicinity of surfaces of materials. In spite of the long history of XPS and its importance in materials science, a general method had not been developed so far to calculate the absolute binding energies for both insulators and metals, including multiple splittings due to chemical shift, spin-orbit coupling, and exchange interaction, on equal footing. In this study, we have developed a novel computational method to calculate absolute binding energies of core levels in metals and insulators, based on a penalty functional and an exact Coulomb cutoff method in a framework of the density functional theory. The spurious interaction of core holes between supercells is avoided by the exact Coulomb cutoff method, while the variational penalty functional enables us to treat multiple splittings due to chemical shift, spin-orbit coupling, and exchange interaction on equal footing, both of which are not accessible by previous methods. It is demonstrated that the absolute binding energies of core levels for both metals and insulators are calculated by the proposed method in a mean absolute (relative) error of 0.4 eV (0.16 %) for eight cases compared to experimental values measured with X-ray photoemission spectroscopy within a generalized gradient approximation to the exchange-correlation functional. We have applied the developed method to silicene grown on  $\text{ZrB}_2$  substrate, which is one of fascinating two-dimensional materials discovered recently. It is found that the obtained binding energies of Si-2p states of the planar structure are in good agreement with the XPS data measured at the photon factory, KEK, resulting in a success of detailed analysis of buckling form of silicene.

1. Electronic transport properties of graphene channel with metal electrodes or insulating substrates in 10 nm-scale devices: H. Jippo, T. Ozaki, S. Okada and M. Ohfuchi, *J. Appl. Phys.* **120** (2016) 154301.
2. Reproducibility in density functional theory calculations of solids: K. Lejaeghere, G. Bihlmayer, T. Bjorkman, P. Blaha, S. Blugel, V. Blum, D. Caliste, I. E. Castelli, S. J. Clark, A. Dal Corso, S. de Gironcoli, T. Deutsch, J. K. Dewhurst, I. Di Marco, C. Draxl, M. Du ak, O. Eriksson, J. A. Flores-Livas, K. F. Garrity, L. Genovese, P. Giannozzi, M. Giantomassi, S. Goedecker, X. Gonze, O. Granas, E. K. U. Gross, A. Gulans, F. Gygi, D. R. Hamann, P. J. Hasnip, N. A. W. Holzwarth, D. Iu an, D. B. Jochym, F. Jollet, D. Jones, G. Kresse, K. Koepernik, E. Kucukbenli, Y. O. Kvasninin, I. L. M. Locht, S. Lubeck, M. Marsman, N. Marzari, U. Nitzsche, L. Nordstrom, T. Ozaki, L. Paulatto, C. J. Pickard, W. Poelmans, M. I. J. Probert, K. Refson, M. Richter, G. -M. Rignanese, S. Saha, M. Scheffler, M. Schlipf, K. Schwarz, S. Sharma, F. Tavazza, P. Thunstrom, A. Tkatchenko, M. Torrent, D. Vanderbilt, M. J. van Setten, V. Van Speybroeck, J. M. Wills, J. R. Yates, G. -X. Zhang and S. Cottenier, *Science* **351** (2016) aad3000(1-7).
3. Hybrid and 4-D FFT implementations of an open-source parallel FFT package OpenFFT: T. V. T. Duy and T. Ozaki, *J Supercomput* **72** (2016) 391-416.
4. \*Single-particle excitation of core states in epitaxial silicene: C.-C. Lee, J. Yoshinobu, K. Mukai, S. Yoshimoto, H. Ueda, A. Fleurence, Y. Yamada-Takamura and T. Ozaki, *Phys. Rev. B* **95** (2017) 115437.
5. Single-particle excitation of core states in epitaxial silicene: C.-C. Lee, J. Yoshinobu, K. Mukai, S. Yoshimoto, H. Ueda, R. Friedlein, A. Fleurence, Y. Yamada-Takamura and T. Ozaki, *Phys. Rev. B* **95** (2017) 115437.
6. Thermoelectric properties of high power factor sulfide  $\text{NiSbS}$  and Co substitution system  $\text{Ni}_{1-x}\text{Co}_x\text{SbS}$ : M. Miyata, T. Ozaki, S. Nishino and M. Koyano, *Jpn. J. Appl. Phys.* **56** (2017) 021801.
7. Absolute Binding Energies of Core Levels in Solids from First Principles: T. Ozaki and C.-C. Lee, *Phys. Rev. Lett.* **118** (2017) 026401.
8. Chemical misfit origin of solute strengthening in iron alloys: M. Wakeda, T. Tsuru, M. Kohyama, T. Ozaki, H. Sawada, M. Itakura and S. Ogata, *Acta Materialia* **131** (2017) 445.

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\* Joint research among groups within ISSP.

# Laser and Synchrotron Research Center

## Shin group

We studied high Tc Fe-pnictide superconductors using 7-eV laser. High resolution photoemission study with polarization dependence is very powerful for the study of the superconducting mechanism. Orbital fluctuation mechanism is also important in addition to the spin fluctuation mechanism.

1. †\* One-dimensional metallic surface states of Pt-induced atomic nanowires on Ge(001): K. Yaji, S. Kim, I. Mochizuki, Y. Takeichi, Y. Ohtsubo, P. L. Fèvre, F. Bertran, A. Taleb-Ibrahimi, S. Shin and F. Komori, *J. Phys.: Condens. Matter* **28** (2016) 284001 (1-9).
2. † Coexistence of a pseudo-gap and a superconducting gap for the high-Tc superconductor LSCO using photoemission spectroscopy: T. Yoshida, W. Malaeb, S. Ideta, D. H. Lu, R. G. Moor, Z. -X. Shen, M. Okawa, T. Kiss, K. Ishizaka, S. Shin, S. Komiya, Y. Ando, H. Eisaki, S. Uchida and A. Fujimori, *Phys. Rev. B* **93** (2016) 014513(5 pages).
3. \* Coherent control over three-dimensional spin polarization for the spin-orbit coupled surface state of Bi<sub>2</sub>Se<sub>3</sub>: K. Kuroda, K. Yaji, M. Nakayama, A. Harasawa, Y. Ishida, S. Watanabe, C. -T. Chen, T. Kondo, F. Komori and S. Shin, *Phys. Rev. B* **94** (2016) 165162(R)(1-5).
4. †\* Fermi arc electronic structure and Chern numbers in the type-II Weyl semimetal candidate Mo<sub>x</sub>W<sub>1-x</sub>Te<sub>2</sub>: I. Belopolski, S. Y. Xu, Y. Ishida, X. Pan, P. Yu, D. S. Sanchez, H. Zheng, M. Neupane, N. Alidoust, G. Chang, T. R. Chang, Y. Wu, G. Bian, S. M. Huang, C. C. Lee, D. Mou, L. Huang, Y. Song, B. Wang, G. Wang, Y. W. Yeh, N. Yao, J. E. Rault, P. L. Fèvre, F. Bertran, H. T. Jeng, T. Kondo, A. Kaminski, H. Lin, Z. Liu, F. Song, S. Shin and M. Z. Hasan, *Phys. Rev. B* **94** (2016) 085127(1-7).
5. † Revealing the ultrafast light-to-matter energy conversion before heat diffusion in a layered Dirac semimetal: Y. Ishida, H. Masuda, H. Sakai, S. Ishiwata and S. Shin, *Phys. Rev. B* **93** (2016) 100302(6 pages).
6. \* Spin texture in type-II Weyl semimetal WTe<sub>2</sub>: B. Feng, Y.-H. Chan, Y. Feng, R.-Y. Liu, M.-Y. Chou, K. Kuroda, K. Yaji, A. Harasawa, P. Moras, A. Barinov, W. Malaeb, C. Bareille, T. Kondo, S. Shin, F. Komori, T.-C. Chiang, Y. Shi and I. Matsuda, *Phys. Rev. B* **94** (2016) 195134(1-5).
7. \* High repetition pump-and-probe photoemission spectroscopy based on a compact fiber laser system: Y. Ishida, T. Otsu, A. Ozawa, K. Yaji, S. Tani, S. Shin and Y. Kobayashi, *Rev. Sci. Instrum.* **87** (2016) 123902(1-11).
8. \* High-resolution three-dimensional spin- and angle-resolved photoelectron spectrometer using vacuum ultraviolet laser light: K. Yaji, A. Harasawa, K. Kuroda, S. Toyohisa, M. Nakayama, Y. Ishida, A. Fukushima, S. Watanabe, C. Chen, F. Komori and S. Shin, *Rev. Sci. Instrum.* **87** (2016) 053111(1-6).
9. †\* Slater to Mott Crossover in the Metal to Insulator Transition of Nd<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub>: M. Nakayama, T. Kondo, Z. Tian, J. J. Ishikawa, M. Halim, C. Bareille, W. Malaeb, K. Kuroda, T. Tomita, S. Ideta, K. Tanaka, M. Matsunami, S. Kimura, N. Inami, K. Ono, H. Kumigashira, L. Balents, S. Nakatsuji and S. Shin, *Phys. Rev. Lett.* **117** (2016) 05640(1-6).
10. †\* Spin Polarization and Texture of the Fermi Arcs in the Weyl Fermion Semimetal TaAs: S.-Y. Xu, I. Belopolski, D. S. Sanchez, M. Neupane, G. Chang, K. Yaji, Z. Yuan, C. Zhang, K. Kuroda, G. Bian, C. Guo, H. Lu, T.-R. Chang, N. Alidoust, H. Zheng, C.-C. Lee, S.-M. Huang, C.-H. Hsu, H.-T. Jeng, A. Bansil, T. Neupert, F. Komori, T. Kondo, S. Shin, H. Lin, S. Jia and M. Zahid Hasan, *Phys. Rev. Lett.* **116** (2016) 096801(1-7).
11. †\* 角度分解光電子分光による精密測定で解き明かす銅酸化物高温超伝導体の擬ギャップと超伝導ギャップの競合関係: 近藤 猛, 竹内 恒博, 辛 埴, *固体物理* **51** (2016) 203-221.
12. 超高速時間分解光電子分光: 石田 行章, *表面科学* **37** (2016) 31-36.
13. Microstructural evolution and correlated magnetic domain configuration of nanoparticles embedded in a single crystal of Cu<sub>75</sub>-Ni<sub>20</sub>-Fe<sub>5</sub> alloy: J.-S. Kim, T. Taniuchi, M. Mizuguchi, S. Shin, K. Takanashi and M. Takeda, *J. Phys. D: Appl. Phys.* **49** (2016) 335006(1-7).
14. Imaging of room-temperature ferromagnetic nano-domains at the surface of a non-magnetic oxide: T. Taniuchi, Y. Motoyui, K. Morozumi, T. C. Rödel, F. Fortuna, A. F. Santander-Syro and S. Shin, *Nat. Commun.* **7** (2016) 11781 (1-6).
15. † Electronic structure and relaxation dynamics in a superconducting topological material: M. Neupane, Y. Ishida, R. Sankar, J.-X. Zhu, D. S. Sanchez, I. Belopolski, S.-Y. Xu, N. Alidoust, M. Mofazzel Hosen, S. Shin, F. Chou, M. Zahid Hasan and T. Durakiewicz, *Sci. Rep.* **6** (2016) 22557(7 pages).

† Joint research with outside partners.

16. † Quasi-particles ultrafastly releasing kink bosons to form Fermi arcs in a cuprate superconductor: Y. Ishida, T. Saitoh, T. Mochiku, T. Nakane, K. Hirata and S. Shin, *Sci. Rep.* **6** (2016) 18747(8 pages).
17. \* Direct mapping of spin and orbital entangled wave functions under interband spin-orbit coupling of giant Rashba spin-split surface states: R. Noguchi, K. Kuroda, K. Yaji, K. Kobayashi, M. Sakano, A. Harasawa, T. Kondo, F. Komori and S. Shin, *Phys. Rev. B* **95** (2017) 041111(R)(1-6).
18. \* Suppression of supercollision carrier cooling in high mobility graphene on SiC(000-1): T. Someya, H. Fukidome, H. Watanabe, T. Yamamoto, M. Okada, H. Suzuki, Y. Ogawa, T. Iimori, N. Ishii, T. Kanai, K. Tashima, B. Feng, S. Yamamoto, J. Itatani, F. Komori, K. Okazaki, S. Shin and I. Matsuda, *Phys. Rev. B* **95** (2017) 165303(1-7).
19. †\* Ultrafast Melting of Spin Density Wave Order in BaFe<sub>2</sub>As<sub>2</sub> Observed by Time- and Angle-Resolved Photoemission Spectroscopy with Extreme-Ultraviolet Higher Harmonic Generation: H. Suzuki, K. Okazaki, T. Yamamoto, T. Someya, M. Okada, K. Koshiishi, M. Fujisawa, T. Kanai, N. Ishii, M. Nakajima, H. Eisaki, K. Ono, H. Kumigashira, J. Itatani, A. Fujimori and S. Shin, *Phys. Rev. B* **95** (2017) 165112(1-6).
20. †\* Unusual nodal behaviors of the superconducting gap in the iron-based superconductor Ba(Fe<sub>0.65</sub>Ru<sub>0.35</sub>)<sub>2</sub>As<sub>2</sub>: Effects of spin-orbit coupling: L. Liu, K. Okazaki, T. Yoshida, H. Suzuki, M. Horio, L. C. C. Ambolode II, J. Xu, S. Ideta, M. Hashimoto, D. H. Lu, Z. -X. Shen, Y. Ota, S. Shin, M. Nakajima, S. Ishida, K. Kihou, C. H. Lee, A. Iyo, H. Eisaki, T. Mikami, T. Kakeshita, Y. Yamakawa, H. Kontani, S. Uchida and A. Fujimori, *Phys. Rev. B* **95** (2017) 104504(1-5).
21. Topologically Entangled Rashba-Split Shockley States on the Surface of Grey Arsenic: P. Zhang, J. -Z. Ma, Y. Ishida, L. -X. Zhao, Q. -N. Xu, B. -Q. Lv, K. Yaji, G. -F. Chen, H. -M. Weng, X. Dai, Z. Fang, X. -Q. Chen, L. Fu, T. Qian, H. Ding and S. Shin, *Phys. Rev. Lett.* **118** (2017) 046802(1-5).
22. \* Capturing ultrafast magnetic dynamics by time-resolved soft x-ray magnetic circular dichroism: K. Takubo, K. Yamamoto, Y. Hirata, Y. Yokoyama, Y. Kubota, S. Yamamoto, S. Yamamoto, I. Matsuda, S. Shin, T. Seki, K. Takanashi and H. Wadati, *Appl. Phys. Lett.* **110** (2017) 162401(1-5).
23. \* Spin-dependent quantum interference in photoemission process from spin-orbit coupled states: K. Yaji, K. Kuroda, S. Toyohisa, A. Harasawa, Y. Ishida, S. Watanabe, C. Chen, K. Kobayashi, F. Komori and S. Shin, *Nat. Commun.* **8** (2017) 14588(1-6).
24. \* Unconventional superconductivity in the BiS<sub>2</sub>-based layered superconductor NdO<sub>0.71</sub>F<sub>0.29</sub>BiS<sub>2</sub>: Y. Ota, K. Okazaki, H. Q. Yamamoto, T. Yamamoto, S. Watanabe, C. Chen, M. Nagao, S. Watauchi, I. Tanaka, Y. Takano and S. Shin, *Phys. Rev. Lett.* **118** (2017) 167002(1-6).
25. \* Polarization dependence of resonant magneto-optical Kerr effect measured by two types of figure-8 undulators: Y. Kubota, Sh. Yamamoto, T. Someya, Y. Hirata, K. Takubo, M. Araki, M. Fujisawa, K. Yamamoto, Y. Yokoyama, M. Taguchi, S. Yamamoto, M. Tsunoda, H. Wadati, S. Shin and I. Matsuda, *J. Elec. Spec. Rel. Phenom* (2016), in print.

## I. Matsuda group

In 2016, we made large progress in research of the novel materials, especially "borophene". We directly observed its metallicity and, moreover, we discovered the Dirac Fermions. It is of note that the borophene we synthesized is the first metal allotrope of boron in a history of the condensed matter physics. Concerning our developments and experiments of the advanced spectroscopies, we successfully achieved in generating new techniques. One of them is to determine the element-specific complex permittivity using a fast-switching undulator that we have developed at SPring-8 BL07LSU. The other is to measure soft X-ray nonlinear effect with a X-ray free electron laser at SACLA. At the end-station of SPring-8 BL07LSU, we upgraded the time-resolved soft X-ray photoemission system by introducing a high-frequency laser. The time-resolved data for joint-researches were improved significantly that has allowed us not only to measure with high-resolution but also to save beamtime and to accept more proposals for our beamline.

1. \* Direct evidence of metallic bands in a monolayer boron sheet: B. Feng, J. Zhang, R.-Y. Liu, T. Iimori, C. Lian, H. Li, L. Chen, K. Wu, S. Meng, F. Komori and I. Matsuda, *Phys. Rev. B* **94** (2016) 041408(1-5).
2. Phonon-dressed two-dimensional carriers on the ZnO surface: R. Yukawa, K. Ozawa, S. Yamamoto, H. Iwasawa, K. Shimada, E. F. Schwier, K. Yoshimatsu, H. Kumigashira, H. Namatame, M. Taniguchi and I. Matsuda, *Phys. Rev. B* **94** (2016) 165313(1-5).
3. \* Spin texture in type-II Weyl semimetal WTe<sub>2</sub>: B. Feng, Y.-H. Chan, Y. Feng, R.-Y. Liu, M.-Y. Chou, K. Kuroda, K. Yaji, A. Harasawa, P. Moras, A. Barinov, W. Malaeb, C. Bareille, T. Kondo, S. Shin, F. Komori, T.-C. Chiang, Y. Shi and I. Matsuda, *Phys. Rev. B* **94** (2016) 195134(1-5).

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\* Joint research among groups within ISSP.

4. †\* Proving Nontrivial Topology of Pure Bismuth by Quantum Confinement: S. Ito, B. Feng, M. Arita, A. Takayama, R. -Y. Liu, T. Someya, W. -C. Chen, T. Iimori, H. Namatame, M. Taniguchi, C. -M. Cheng, S. -J. Tang, F. Komori, K. Kobayashi, T. -C. Chiang and I. Matsuda, *Phys. Rev. Lett.* **117** (2016) 236402(1-5).
5. Generation of metallic  $e_g$ -derived band at Cs/SrTiO<sub>3</sub> interface observed by polarization-dependent photoemission spectroscopy: K. Akikubo, I. Matsuda, D. Schmaus, G. Marcaud, S. Yamamoto, R.-Y. Liu, R. Yukawa, M. G. Silly, F. Sirotti and M. D'Angelo, *Thin Solid Films* **603** (2016) 149-153.
6. 時間分解軟X線光電子分光法:半導体表面における光励起キャリアの実時間観測: 山本 達, 松田 巖, *表面科学* **37** (2016) 9-13.
7. What Determines the Lifetime of Photoexcited Carriers on TiO<sub>2</sub> Surfaces?: K. Ozawa, S. Yamamoto, R. Yukawa, R. -Y. Liu, M. Emori, K. Inoue, T. Higuchi, H. Sakama, K. Mase and I. Matsuda, *J. Phys. Chem. C* **120** (2016) 29283-29289.
8. Capturing transient charged states at the C<sub>60</sub>/TiO<sub>2</sub>(110) interface by time-resolved soft X-ray photoelectron spectroscopy: K. Ozawa, S. Yamamoto, R. Yukawa, K. Akikubo, M. Emori, H. Sakama and I. Matsuda, *Organic Electronics* **31** (2016) 98-103.
9. Microscopic observation and chemical mapping of opal phytoliths in a mulberry leaf: O. Tsutsui, R. Sakamoto, M. Hattori, K. Hasegawa, T. Handa, D. Nishio-Hamane and I. Matsuda, *Flora* **218** (2016) 44-50.
10. \* Real-time observation of reaction processes of CO<sub>2</sub> on Cu(997) by ambient-pressure X-ray photoelectron spectroscopy: T. Koitaya, S. Yamamoto, Y. Shiozawa, K. Takeuchi, R.-Y. Liu, K. Mukai, S. Yoshimoto, K. Akikubo, I. Matsuda and J. Yoshinobu, *Topic in Catalysis* **59** (2016) 526-531.
11. Structure determination of germanene on an Al(111) surface using total-reflection high-energy positron diffraction: Y. Fukaya, I. Matsuda, B. Feng I. Mochizuki, T. Hyodo and S. Shamoto, *2D Materials* **3** (2016) 035019(1-7).
12. Tailoring photovoltage response at SrRuO<sub>3</sub>/SrTiO<sub>3</sub> heterostructures: R. Yukawa, S. Yamamoto, K. Akikubo, K. Takeuchi, K. Ozawa, H. Kumigashira and I. Matsuda, *Adv. Mat. Interfaces* **3** (2016) 1600527(1-5).
13. \* Surface state of the dual topological insulator Bi Sb (112): I. Matsuda, K. Yaji, A. A. Taskin, M. D'angelo, R. Yukawa, Y. Ohtsubo, P. Le Fèvre, F. Bertran, S. Yoshizawa, A. Taleb-Ibrahimi, A. Kakizaki, Y. Ando and F. Komori, *Physica B* **516** (2017) 100-104.
14. \* Suppression of supercollision carrier cooling in high mobility graphene on SiC(000-1): T. Someya, H. Fukidome, H. Watanabe, T. Yamamoto, M. Okada, H. Suzuki, Y. Ogawa, T. Iimori, N. Ishii, T. Kanai, K. Tashima, B. Feng, S. Yamamoto, J. Itatani, F. Komori, K. Okazaki, S. Shin and I. Matsuda, *Phys. Rev. B* **95** (2017) 165303(1-7).
15. †\* Dirac Fermions in Borophene: B. Feng, O. Sugino, R.-Y. Liu, J. Zhang, R. Yukawa, M. Kawamura, T. Iimori, H. Kim, Y. Hasegawa, H. Li, L. Chen, K. Wu, H. Kumigashira, F. Komori, T.-C. Chiang, S. Meng and I. Matsuda, *Phys. Rev. Lett.* **118** (2017) 096401(1-6).
16. \* Capturing ultrafast magnetic dynamics by time-resolved soft x-ray magnetic circular dichroism: K. Takubo, K. Yamamoto, Y. Hirata, Y. Yokoyama, Y. Kubota, S. Yamamoto, S. Yamamoto, I. Matsuda, S. Shin, T. Seki, K. Takanashi and H. Wadati, *Appl. Phys. Lett.* **110** (2017) 162401(1-5).
17. Time-resolved soft X-ray core-level photoemission spectroscopy to 880°C using pulsed laser and synchrotron radiation, and switched heating current: T. Abukawa, S. Yamamoto, R. Yukawa, S. Kanzaki, K. Mukojima and I. Matsuda, *Surf. Sci.* **656** (2017) 43-47.
18. \* Adsorption of CO<sub>2</sub> on Graphene: A Combined TPD, XPS, and vdW-DF Study: K. Takeuchi, S. Yamamoto, Y. Hamamoto, Y. Shiozawa, K. Tashima, H. Fukidome, T. Koitaya, K. Mukai, S. Yoshimoto, M. Suemitsu, Y. Morikawa, J. Yoshinobu and I. Matsuda, *J. Phys. Chem. C* **121** (2017) 2807.
19. \* CO<sub>2</sub> adsorption on graphene studied by TPD and DFT calculation with van der Waals density functional: K. Takeuchi, S. Yamamoto, Y. Hamamoto, Y. Shiozawa, K. Tashima, H. Fukidome, T. Koitaya, K. Mukai, S. Yoshimoto, M. Suemitsu, Y. Morikawa, J. Yoshinobu and I. Matsuda, *J. Phys. Chem. C* **121** (2017) 2807-2814.
20. \* Interface Electronic Structure at the Topological Insulator-Ferrimagnetic Insulator Junction: Y. Kubota, K. Murata, J. Miyawaki, K. Ozawa, M. Onbasli, T. Shirasawa, B. Feng, Sh. Yamamoto, R.-Y. Liu, S. Yamamoto, S. Mahatha, P. Sheverdyevaeva, P. Moras, C. Ross, S. Suga, Y. Harada, K. Wang and I. Matsuda, *J. Phys. Condens. Matter* **29** (2017) 055002(1-6).
21. \* Polarization dependence of resonant magneto-optical Kerr effect measured by two types of figure-8 undulators: Y. Kubota, Sh. Yamamoto, T. Someya, Y. Hirata, K. Takubo, M. Araki, M. Fujisawa, K. Yamamoto, Y. Yokoyama, M. Taguchi, S. Yamamoto, M. Tsunoda, H. Wadati, S. Shin and I. Matsuda, *J. Elec. Spec. Rel. Phenom* (2016), in print.

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† Joint research with outside partners.

22. \* ホウ素単原子シート「ボロフェン」：金属性とディラックフェルミオン：F. Baojie, 松田 巖, 固体物理 (2017), in print.

## Kobayashi group

We are developing a high-average-power, femtosecond laser system with Yb-doped fibers. Average power of 100 W is achieved.

1. \* High repetition pump-and-probe photoemission spectroscopy based on a compact fiber laser system: Y. Ishida, T. Otsu, A. Ozawa, K. Yaji, S. Tani, S. Shin and Y. Kobayashi, *Rev. Sci. Instrum.* **87** (2016) 123902(1-11).
2. 10GHz を超える高繰り返し光周波数コム：遠藤 護, 小林 洋平, 光学 **45** (2016) 271-273.
3. Ytterbium fiber-based, 270 fs, 100 W chirped pulse amplification laser system with 1 MHz repetition rate: Z. Zhao and Y. Kobayashi, *Appl. Phys. Express* **9** (2016) 012701(1-4).
4. Wavelength-spacing controllable, dual-wavelength synchronously mode locked Er: fiber laser oscillator based on dual-branch nonlinear polarization rotation technique: S. Wang, Z. Zhao and Y. Kobayashi, *Opt. Express* **24** (2016) 28228-28238.
5. \* High-precision group-delay dispersion measurements of optical fibers via fingerprint-spectral wavelength-to-time mapping: T. Ito, O. Slezak, M. Yoshita, H. Akiyama and Y. Kobayashi, *Photon. Res.* **4** (2016) 13-16.
6. Phase-matched frequency conversion below 150 nm in  $\text{KBe}_2\text{BO}_3\text{F}_2$ : T. Nakazato, I. Ito, Y. Kobayashi, X. Wang, C. Chen and S. Watanabe, *Optics Express* **24** (2016) 17149-17158.
7. Kerr-lens mode-locked bidirectional dual-comb ring laser for broadband dual-comb spectroscopy: T. Ideguchi, T. Nakamura, Y. Kobayashi and K. Goda, *Optica* **3** (2016) 748-753.
8. Magneto-optic modulator for high bandwidth cavity length stabilization: T. Nakamura, S. Tani, I. Ito and Y. Kobayashi, *Optics Express* **25** (2017) 4994-5000.
9. 149.8 nm, the shortest wavelength generated by phase matching in nonlinear crystals: T. Nakazato, I. Ito, Y. Kobayashi, X. Wang, C. Chen and S. Watanabe, in: *Proc. SPIE 10088, Nonlinear Frequency Generation and Conversion: Materials and Devices XVI* (SPIE, 2017), 1008804(1-10).
10. 先端レーザー技術の産業展開：小林 洋平, 趙 智剛, 谷峻 太郎, 月刊 OPTRONICS **35-418** (2016) 60-65.
11. ファイバーレーザーベース狭帯域 193nm 固体レーザーの開発：伊藤 紳二, 玄 洪文, 五十嵐 裕紀, 趙 智剛, 小林 洋平, 光学 第 46 巻第 4 号 (2017) 125-130.

## Itatani group

First, we continued the development of intense ultrafast MIR sources based on optical parametric amplification (OPA). One source was BIBO-based OPA followed by difference frequency generation, which covered the spectral range in 5-10  $\mu\text{m}$ . Another source was KTA-based OPA that produced 100-% $\mu\text{J}$ , 100-fs pulses at 3.2  $\mu\text{m}$ . Both sources had stable carrier-envelope phases (CEPs), and were used to study high harmonic generation (HHG) in crystalline solids. Polarization-resolved spectroscopy revealed the generation process of solid HHG where carrier transport in band structures played a significant role. Nanotip experiments were also carried out with the MIR sources. We confirmed the plasmonic field enhancement by photoelectron measurement. Second, we continued strong field experiments using a BIBO-based optical parametric chirped pulse amplifier that routinely produced CEP-stable, 1.5-mJ, 10-fs pulses at 1.7 $\mu\text{m}$  with a repetition rate of 1 kHz. Attosecond streaking measurement was achieved where diffuse atoms were ionized by an attosecond XUV pulse and a CEP-stable IR field. Generation of isolated 450-attosecond pulses at 100 eV was experimentally confirmed. This is the first attosecond streaking measurement using an OPCPA-based infrared source, showing the capability of IR-OPCPA to extend the attosecond methodology from XUV (<200 eV) to soft-X-ray (>200 eV) regions. Such energy upscale is needed to realize ultrafast soft-X-ray spectroscopy in future. We also started to develop a novel velocity-map-imaging photoelectron spectrometer under the collaboration with Prof. Kling group in Germany. This apparatus is designed to measure the momentum distribution of photoelectrons up to 2 keV, which will be used to explore high-energy attosecond processes induced by long-wavelength optical fields.

1. † Carrier-envelope phase mapping in laser-induced electron diffraction: H. Geiseler, N. Ishii, K. Kaneshima, F. Geier, T. Kanai, O. I. Tolstikhin, T. Morishita and J. Itatani, *Phys. Rev. A* **94** (2016) 033417.
2. Generation of carrier-envelope phase-stable mid-infrared pulses via dual-wavelength optical parametric amplification: K. Kaneshima, N. Ishii, K. Takeuchi and J. Itatani, *Opt. Express* **24** (2016) 8660(1-6).
3. † Attosecond streaking measurement of extreme ultraviolet pulses using a long-wavelength electric field: N. Saito, N. Ishii, T. Kanai, S. Watanabe and J. Itatani, *Sci. Rep.* **6** (2016) 35594(1-5).

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\* Joint research among groups within ISSP.

4. Generation of spectrally stable 6.5-fs visible pulses via filamentation in krypton: K. Kaneshima, K. Takeuchi, N. Ishii and J. Itatani, *High Power Laser Science and Engineering* **4** (2016) e17(1-5).
5. \*Suppression of supercollision carrier cooling in high mobility graphene on SiC(000-1): T. Someya, H. Fukidome, H. Watanabe, T. Yamamoto, M. Okada, H. Suzuki, Y. Ogawa, T. Iimori, N. Ishii, T. Kanai, K. Tashima, B. Feng, S. Yamamoto, J. Itatani, F. Komori, K. Okazaki, S. Shin and I. Matsuda, *Phys. Rev. B* **95** (2017) 165303(1-7).
6. †\*Ultrafast Melting of Spin Density Wave Order in BaFe<sub>2</sub>As<sub>2</sub> Observed by Time- and Angle-Resolved Photoemission Spectroscopy with Extreme-Ultraviolet Higher Harmonic Generation: H. Suzuki, K. Okazaki, T. Yamamoto, T. Someya, M. Okada, K. Koshiishi, M. Fujisawa, T. Kanai, N. Ishii, M. Nakajima, H. Eisaki, K. Ono, H. Kumigashira, J. Itatani, A. Fujimori and S. Shin, *Phys. Rev. B* **95** (2017) 165112(1-6).

## Harada group

Integrating the ambient pressure setup using a differential pumping system realized by FY2015, micro-focusing of the X-ray beam using KB mirrors, and angle resolved mode using the newly developed rotation chamber, we realized the following soft X-ray resonant inelastic X-ray scattering (RIXS) experiments in FY2016. (A) Observation of two-dimensional (excitation energy and momentum) mapping of RIXS By optimizing the focusing optics and using the horizontal rotation of the RIXS spectrometer, angle resolved soft X-ray RIXS spectra of high T<sub>c</sub> cuprates were obtained across O 1s resonance, which provides unique information about the Cu-O mixing and resultant dispersion from the oxygen side. (B) Combined use of soft X-ray diffraction and RIXS using the angle resolved system High resolution angle resolved RIXS enables us combined use of soft X-ray diffraction from the elastic part and soft X-ray RIXS from the inelastic part. The first demonstration of such experiment was performed for LaSrFeO<sub>4</sub> which is well known to exhibit orbital ordering. Spatial modulation of the electron density yields not only soft X-ray diffraction but also intensity modulation of RIXS by the scattering angle, showing possibility of measuring ‘inelastic X-ray diffraction’. This year we have accepted 14 collaborative works at BL07LSU HORNET endstation, which include the above two topics and study on water encapsulated in polymers, bio-inspired materials, humidity dependence of functional transition metal complexes and operando analysis of Li ion battery electrodes.

1. †Hybridization and electron-phonon coupling in ferroelectric BaTiO<sub>3</sub> probed by resonant inelastic x-ray scattering: S. Fatale, S. Moser, J. Miyawaki, Y. Harada and M. Grioni, *Phys. Rev. B* **94** (2016) 195131(1-6).
2. †Resonant inelastic x-ray scattering study of entangled spin-orbital excitations in superconducting PrFeAsO<sub>0.7</sub>: T. Nomura, Y. Harada, H. Niwa, K. Ishii, M. Ishikado, S. Shamoto and I. Jarrige, *Phys. Rev. B* **94** (2016) 035134(1-9).
3. †Redox Potential Paradox in Na<sub>x</sub>MO<sub>2</sub> for Sodium-Ion Battery Cathodes: Y. Nanba, T. Iwao, B. M. D. Boisse, W. Zhao, E. Hosono, D. Asakura, H. Niwa, H. Kiuchi, J. Miyawaki, Y. Harada, M. Okubo and A. Yamada, *Chem. Mater.* **28** (2016) 1058-1065.
4. †Combined Experimental and Computational Analyses on the Electronic Structure of Alluaudite-Type Sodium Iron Sulfate: G. Oyama, H. Kiuchi, S. C. Chung, Y. Harada and A. Yamada, *J. Phys. Chem. C* **120** (2016) 23323-23328.
5. In Situ Hard X-ray Photoelectron Study of O<sub>2</sub> and H<sub>2</sub>O Adsorption on Pt Nanoparticles: Y. Cui, Y. Harada, E. Ikenaga, R. Li, N. Nakamura, T. Hatanaka, M. Ando, T. Yoshida, G.-L. Li and M. Oshima, *J. Phys. Chem. C* **120** (2016) 10936-10940.
6. †Characterization of nitrogen species incorporated into graphite using low energy nitrogen ion sputtering: H. Kiuchi, T. Kondo, M. Sakurai, D. Guo, J. Nakamura, H. Niwa, J. Miyawaki, M. Kawai, M. Oshima and Y. Harada, *Phys. Chem. Chem. Phys.* **18** (2016) 458-465.
7. †Intermediate honeycomb ordering to trigger oxygen redox chemistry in layered battery electrode: B. M. D. Boisse, G. Liu, J. Ma, S.-I. Nishimura, S.-C. Chung, H. Kiuchi, Y. Harada, J. Kikkawa, Y. Kobayashi, M. Okubo and A. Yamada, *Nat. Commun.* **7** (2016) 11397(1-9).
8. Pt-free carbon-based fuel cell catalyst prepared from spherical polyimide for enhanced oxygen diffusion: Y. Nabae, S. Nagata, T. Hayakawa, H. Niwa, Y. Harada, M. Oshima, A. Isoda, A. Matsunaga, K. Tanaka and T. Aoki, *Sci. Rep.* **6** (2016) 23276(1-7).
9. †Lewis Basicity of Nitrogen-Doped Graphite Observed by CO<sub>2</sub> Chemisorption: H. Kiuchi, R. Shibuya, T. Kondo, J. Nakamura, H. Niwa, J. Miyawaki, M. Kawai, M. Oshima and Y. Harada, *Nanoscale Res Lett* **11** (2016) 127(1-7).
10. Electronic Structure of Pt and Pt-Co Nanoparticles with O<sub>2</sub> and O<sub>2</sub>/H<sub>2</sub>O Adsorption Revealed by In Situ XAFS and Hard X-Ray Photoelectron Spectroscopy: Y. -T. Cui, Y. Harada, T. Hatanaka, N. Nakamura, M. Ando, T. Yoshida, E. Ikenaga, K. Ishii, D. Matsumura, R. Li and M. Oshima, *ECS Transactions* **72** (2016) 131-136.
11. †X-ray and Electron Spectroscopy of Water: T. Fransson, Y. Harada, N. Kosugi, N. A. Besley, B. Winter, J. J. Rehr, L. G. M. Pettersson and A. Nilsson, *Chem. Rev.* **116** (2016) 7551-7569.

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† Joint research with outside partners.

- \* Interface Electronic Structure at the Topological Insulator-Ferrimagnetic Insulator Junction: Y. Kubota, K. Murata, J. Miyawaki, K. Ozawa, M. Onbasli, T. Shirasawa, B. Feng, Sh. Yamamoto, R.-Y. Liu, S. Yamamoto, S. Mahatha, P. Sheverdyaeva, P. Moras, C. Ross, S. Suga, Y. Harada, K. Wang and I. Matsuda, *J. Phys. Condens. Matter* **29** (2017) 055002(1-6).

## Wadati group

We succeeded in the observation of photoinduced demagnetization and insulator-to-metal transition in ferromagnetic insulating BaFeO<sub>3</sub> thin films by time-resolved x-ray magnetic circular dichroism. We also studied the thickness-dependent physical properties of La<sub>1/3</sub>Sr<sub>2/3</sub>FeO<sub>3</sub> thin films to obtain critical thickness for charge ordering.

- Thickness-dependent physical properties of La<sub>1/3</sub>Sr<sub>2/3</sub>FeO<sub>3</sub> thin films grown on SrTiO<sub>3</sub> (001) and (111) substrates: M. Minohara, M. Kitamura, H. Wadati, H. Nakao, R. Kumai, Y. Murakami and H. Kumigashira, *J. Appl. Phys.* **120** (2016) 025303(1-6).
- Photoinduced Demagnetization and Insulator-to-Metal Transition in Ferromagnetic Insulating BaFeO<sub>3</sub> Thin Films: T. Tsuyama, S. Chakraverty, S. Macke, N. Pontius, C. Schüßler-Langeheine, H. Y. Hwang, Y. Tokura and H. Wadati, *Phys. Rev. Lett.* **116** (2016) 256402(1-5).
- 新型スピントロニクスと悪魔の階段：和達 大樹，*パリティ* **31** (2016) 48-51.
- Material/element-dependent fluorescence-yield modes on soft X-ray absorption spectroscopy of cathode materials for Li-ion batteries: D. Asakura, E. Hosono, Y. Nanba, H. Zhou, J. Okabayashi, C. Ban, P. -A. Glans, J. Guo, T. Mizokawa, G. Chen, A. J. Achkar, D. G. Hawthorn, T. Z. Regier and H. Wadati, *AIP Advances* **6** (2016) 035105(1-8).
- 時間分解 X 線回折・分光で見た遷移金属化合物：和達 大樹，*固体物理* **52(5)** (2017) 45-53.
- \* Capturing ultrafast magnetic dynamics by time-resolved soft x-ray magnetic circular dichroism: K. Takubo, K. Yamamoto, Y. Hirata, Y. Yokoyama, Y. Kubota, S. Yamamoto, S. Yamamoto, I. Matsuda, S. Shin, T. Seki, K. Takanashi and H. Wadati, *Appl. Phys. Lett.* **110** (2017) 162401(1-5).
- Resonant Soft X-Ray Scattering Studies of Transition-Metal Oxides: H. Wadati, *Springer Tracts in Modern Physics* **269** (2017) 159-196.
- Electronic Structures of SrIrO<sub>3</sub>/SrTiO<sub>3</sub> Superlattices Revealed by Synchrotron X-Ray Diffraction and Spectroscopy: H. Wadati, S. Yamamura, K. Ishii, M. Suzuki, E. Ikenaga, J. Matsuno and H. Takagi, *Adv. X-Ray. Chem. Anal., Japan* **48** (2017) 215-223.
- \* Polarization dependence of resonant magneto-optical Kerr effect measured by two types of figure-8 undulators: Y. Kubota, Sh. Yamamoto, T. Someya, Y. Hirata, K. Takubo, M. Araki, M. Fujisawa, K. Yamamoto, Y. Yokoyama, M. Taguchi, S. Yamamoto, M. Tsunoda, H. Wadati, S. Shin and I. Matsuda, *J. Elec. Spec. Rel. Phenom* (2016), in print.

## Kondo group

We use angle-resolved photoemission spectroscopy (ARPES) with ultrahigh energy resolution. The main findings in 2016 are as follows: (1) Slater to Mott Crossover in the Metal to Insulator Transition of Nd<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub>, (2) Orbital-Dependent Band Narrowing on the Topmost Layer of Sr<sub>2</sub>RuO<sub>4</sub>, and (3) Coherent control over three-dimensional spin polarization for the spin-orbit coupled surface state of Bi<sub>2</sub>Se<sub>3</sub>.

- \* Coherent control over three-dimensional spin polarization for the spin-orbit coupled surface state of Bi<sub>2</sub>Se<sub>3</sub>: K. Kuroda, K. Yaji, M. Nakayama, A. Harasawa, Y. Ishida, S. Watanabe, C. -T. Chen, T. Kondo, F. Komori and S. Shin, *Phys. Rev. B* **94** (2016) 165162(R)(1-5).
- †\* Fermi arc electronic structure and Chern numbers in the type-II Weyl semimetal candidate Mo<sub>x</sub>W<sub>1-x</sub>Te<sub>2</sub>: I. Belopolski, S. Y. Xu, Y. Ishida, X. Pan, P. Yu, D. S. Sanchez, H. Zheng, M. Neupane, N. Alidoust, G. Chang, T. R. Chang, Y. Wu, G. Bian, S. M. Huang, C. C. Lee, D. Mou, L. Huang, Y. Song, B. Wang, G. Wang, Y. W. Yeh, N. Yao, J. E. Rault, P. L. F. evre, F. Bertran, H. T. Jeng, T. Kondo, A. Kaminski, H. Lin, Z. Liu, F. Song, S. Shin and M. Z. Hasan, *Phys. Rev. B* **94** (2016) 085127(1-7).
- \* Spin texture in type-II Weyl semimetal WTe<sub>2</sub>: B. Feng, Y.-H. Chan, Y. Feng, R.-Y. Liu, M.-Y. Chou, K. Kuroda, K. Yaji, A. Harasawa, P. Moras, A. Barinov, W. Malaeb, C. Bareille, T. Kondo, S. Shin, F. Komori, T.-C. Chiang, Y. Shi and I. Matsuda, *Phys. Rev. B* **94** (2016) 195134(1-5).

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\* Joint research among groups within ISSP.

4. \*High-resolution three-dimensional spin- and angle-resolved photoelectron spectrometer using vacuum ultraviolet laser light: K. Yaji, A. Harasawa, K. Kuroda, S. Toyohisa, M. Nakayama, Y. Ishida, A. Fukushima, S. Watanabe, C. Chen, F. Komori and S. Shin, *Rev. Sci. Instrum.* **87** (2016) 053111(1-6).
5. Generation of Transient Photocurrents in the Topological Surface State of  $\text{Sb}_2\text{Te}_3$  by Direct Optical Excitation with Midinfrared Pulses: K. Kuroda, J. Reimann, J. Gdde and U. Hfer, *Phys. Rev. Lett.* **116** (2016) 076801.
6. Orbital-Dependent Band Narrowing Revealed in an Extremely Correlated Hund's Metal Emerging on the Topmost Layer of  $\text{Sr}_2\text{RuO}_4$ : T. Kondo, M. Ochi, M. Nakayama, H. Taniguchi, S. Akebi, K. Kuroda, M. Arita, S. Sakai, H. Namatame, M. Taniguchi, Y. Maeno, R. Arita and S. Shin, *Phys. Rev. Lett.* **117** (2016) 056403.
7. <sup>†\*</sup>Slater to Mott Crossover in the Metal to Insulator Transition of  $\text{Nd}_2\text{Ir}_2\text{O}_7$ : M. Nakayama, T. Kondo, Z. Tian, J. J. Ishikawa, M. Halim, C. Bareille, W. Malaeb, K. Kuroda, T. Tomita, S. Ideta, K. Tanaka, M. Matsunami, S. Kimura, N. Inami, K. Ono, H. Kumigashira, L. Balents, S. Nakatsuji and S. Shin, *Phys. Rev. Lett.* **117** (2016) 05640(1-6).
8. <sup>†\*</sup>Spin Polarization and Texture of the Fermi Arcs in the Weyl Fermion Semimetal TaAs: S.-Y. Xu, I. Belopolski, D. S. Sanchez, M. Neupane, G. Chang, K. Yaji, Z. Yuan, C. Zhang, K. Kuroda, G. Bian, C. Guo, H. Lu, T.-R. Chang, N. Alidoust, H. Zheng, C.-C. Lee, S.-M. Huang, C.-H. Hsu, H.-T. Jeng, A. Bansil, T. Neupert, F. Komori, T. Kondo, S. Shin, H. Lin, S. Jia and M. Zahid Hasan, *Phys. Rev. Lett.* **116** (2016) 096801(1-7).
9. <sup>†\*</sup>角度分解光電子分光による精密測定で解き明かす銅酸化物高温超伝導体の擬ギャップと超伝導ギャップの競合関係：近藤 猛，竹内 恒博，辛 埴，*固体物理* **51** (2016) 203-221.
10. \*Direct mapping of spin and orbital entangled wave functions under interband spin-orbit coupling of giant Rashba spin-split surface states: R. Noguchi, K. Kuroda, K. Yaji, K. Kobayashi, M. Sakano, A. Harasawa, T. Kondo, F. Komori and S. Shin, *Phys. Rev. B* **95** (2017) 041111(R)(1-6).
11. Ultrafast energy- and momentum-resolved surface Dirac photocurrents in the topological insulator  $\text{Sb}_2\text{Te}_3$ : K. Kuroda, J. Reimann, K. A. Kokh, O. E. Tereshchenko, A. Kimura, J. Gdde and U. Hfer, *Phys. Rev. B* **95** (2017) 081103(R).
12. \*Spin-dependent quantum interference in photoemission process from spin-orbit coupled states: K. Yaji, K. Kuroda, S. Toyohisa, A. Harasawa, Y. Ishida, S. Watanabe, C. Chen, K. Kobayashi, F. Komori and S. Shin, *Nat. Commun.* **8** (2017) 14588(1-6).

## Okazaki group

We have investigated superconducting-gap structures of unconventional superconductors such as iron-based superconductors and BiS<sub>2</sub>-based superconductors by a low-temperature and high-resolution laser ARPES apparatus and transient electronic structures in photo-excited non-equilibrium states by a time-resolved ARPES apparatus using EUV and SX lasers. In the fiscal year 2016, we have revealed unconventional superconductivity in  $\text{NdO}_{0.71}\text{F}_{0.29}\text{BiS}_2$  from its quite anisotropic superconducting gap structure, and importance of the spin-orbit coupling for the superconducting gap anisotropy of  $\text{Ba}(\text{Fe}_{0.65}\text{Ru}_{0.35})_2\text{As}_2$ . In addition, we have observed ultrafast melting of the spin density wave order in  $\text{BaFe}_2\text{As}_2$  and a photo-induced excitonic-insulator-to-semimetal transition in  $\text{Ta}_2\text{NiSe}_5$ .

1. Suppression of the antiferromagnetic pseudogap in the electron-doped high-temperature superconductor by protect annealing: M. Horio, T. Adachi, Y. Mori, A. Takahashi, T. Yoshida, H. Suzuki, L. C. C. Ambolode, K. Okazaki, K. Ono, H. Kumigashira, H. Anzai, M. Arita, H. Namatame, M. Taniguchi, D. Ootsuki, K. Sawada, M. Takahashi, T. Mizokawa, Y. Koike and A. Fujimori, *Nat. Commun.* **7** (2016) 10567(1-8).
2. \*Suppression of supercollision carrier cooling in high mobility graphene on SiC(000-1): T. Someya, H. Fukidome, H. Watanabe, T. Yamamoto, M. Okada, H. Suzuki, Y. Ogawa, T. Iimori, N. Ishii, T. Kanai, K. Tashima, B. Feng, S. Yamamoto, J. Itatani, F. Komori, K. Okazaki, S. Shin and I. Matsuda, *Phys. Rev. B* **95** (2017) 165303(1-7).
3. <sup>†\*</sup>Ultrafast Melting of Spin Density Wave Order in  $\text{BaFe}_2\text{As}_2$  Observed by Time- and Angle-Resolved Photoemission Spectroscopy with Extreme-Ultraviolet Higher Harmonic Generation: H. Suzuki, K. Okazaki, T. Yamamoto, T. Someya, M. Okada, K. Koshiishi, M. Fujisawa, T. Kanai, N. Ishii, M. Nakajima, H. Eisaki, K. Ono, H. Kumigashira, J. Itatani, A. Fujimori and S. Shin, *Phys. Rev. B* **95** (2017) 165112(1-6).
4. <sup>†\*</sup>Unusual nodal behaviors of the superconducting gap in the iron-based superconductor  $\text{Ba}(\text{Fe}_{0.65}\text{Ru}_{0.35})_2\text{As}_2$ : Effects of spin-orbit coupling: L. Liu, K. Okazaki, T. Yoshida, H. Suzuki, M. Horio, L. C. C. Ambolode II, J. Xu, S. Ideta, M. Hashimoto, D. H. Lu, Z. -X. Shen, Y. Ota, S. Shin, M. Nakajima, S. Ishida, K. Kihou, C. H. Lee, A. Iyo, H. Eisaki, T. Mikami, T. Kakeshita, Y. Yamakawa, H. Kontani, S. Uchida and A. Fujimori, *Phys. Rev. B* **95** (2017) 104504(1-5).
5. \*Unconventional superconductivity in the BiS<sub>2</sub>-based layered superconductor  $\text{NdO}_{0.71}\text{F}_{0.29}\text{BiS}_2$ : Y. Ota, K. Okazaki, H. Q. Yamamoto, T. Yamamoto, S. Watanabe, C. Chen, M. Nagao, S. Watauchi, I. Tanaka, Y. Takano and S. Shin, *Phys. Rev. Lett* **118** (2017) 167002(1-6).

<sup>†</sup> Joint research with outside partners.