

# Publications

## Division of New Materials 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 2013 include: (1) Investigation by  $^7\text{Li}$ -NMR of the magnetic phase transition in the frustrated antiferromagnets  $\text{LiInCr}_4\text{O}_8$  and  $\text{LiGaCr}_4\text{O}_8$  with the novel breathing pyrochlore structure, (2) Microscopic examination of the quantum critical and non-fermi liquid behavior in the valence fluctuating Yb compound  $\alpha$ - and  $\beta$ - $\text{YbAlB}_4$ , (3) Continued investigation of the magnetic and structural transition in single crystals of volborthite with the distorted Kagome lattice aimed at the full understanding of the phase diagram in magnetic field.

1.  $^\dagger$  Anisotropic spin fluctuations in the quasi one-dimensional frustrated magnet  $\text{LiCuVO}_4$ : K. Nawa, M. Takigawa, M. Yoshida and K. Yoshimura, *J. Phys. Soc. Jpn.* **86** (2013) 094709(1-13).
2.  $^*$  Magnetic Order in the Spin-1/2 Kagome Antiferromagnet Vesignieite: M. Yoshida, Y. Okamoto, M. Takigawa and Z. Hiroi, *J. Phys. Soc. Jpn.* **82** (2013) 013702(1-5).
3.  $^*$  Incomplete Devil's Staircase in the Magnetization Curve of  $\text{SrCu}_2(\text{BO}_3)_2$ : M. Takigawa, M. Horvatic, T. Waki, S. Kramer, C. Berthier, F. L. Bertrand, I. Sheikin, H. Kageyama, Y. Ueda and F. Mila, *Phys. Rev. Lett.* **110** (2013) 067210(1-5).
4. Iterative deconvolution of quadrupole split NMR spectra: F. Mila and M. Takigawa, *Eur. Phys. J. B* **86** (2013) 354(1-4).
5.  $^\dagger^*$  Field-induced incommensurate phase in the strong-rung spin ladder with ferromagnetic legs: H. Yamaguchi, H. Miyagai, M. Yoshida, M. Takigawa, K. Iwase, T. Ono, N. Kase, K. Araki, S. Kittaka, T. Sakakibara, T. Shimokawa, T. Okubo, K. Okunishi, A. Matsuo and Y. Hosokoshi, *Phys. Rev. B* **89** (2014) 220402.

### 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 2013. (1) Field and temperature variations of the specific heat  $C(H,T)$  of the iron pnictide superconductor  $\text{KFe}_2\text{As}_2$  ( $T_c=3.4$  K) were examined at temperatures down to 100 mK. Thermodynamic evidence for the presence of line nodes is obtained from the square-root  $H$  dependence of  $C/T$  in the low- $T$  and low- $H$  regime. Under a magnetic field rotated within the tetragonal  $ab$  plane, a fourfold oscillation is observed in  $C$  and its sign changes at  $0.08 T_c$ . The results indicate that line nodes exist on the superconducting gap where the Fermi velocity is parallel to  $[100]$  directions. (2) We measured the temperature dependence of the magnetization  $M(T)$  of a  $S=1/2$  one dimensional Heisenberg antiferromagnet  $\text{CuPzN}$  (interaction parameter  $J\sim 10$  K) near the saturation field  $H_s\sim 14$  T where a quantum phase transition from a Luttinger liquid ground state to a fully polarized state occurs. It is found that  $M(T)$  at  $H_s$  exhibits a square-root  $T$  dependence below  $\sim 1$  K down to 80 mK, in good agreement with a prediction of the exact solutions.

1. Anomalous Field-Angle Dependence of the Specific Heat of Heavy-Fermion Superconductor  $\text{UPt}_3$ : S. Kittaka, K. An, T. Sakakibara, Y. Haga, E. Yamamoto, N. Kimura, Y. Onuki and K. Machida, *J. Phys. Soc. Jpn.* **82** (2013) 024707(1-5).
2.  $^\dagger$  Coexistence of Ising and XY Spin Systems on a Single Tb Atom in  $\text{TbCoGa}_5$ : N. Sanada, Y. Amou, R. Watanuki, K. Suzuki, I. Yamamoto, H. Mitamura, T. Sakakibara, M. Akatsu, Y. Nemoto and T. Goto, *J. Phys. Soc. Jpn.* **82** (2013) 044713(1-7).
3.  $^*$  Evidence of a High-Field Phase in  $\text{PrV}_2\text{Al}_{20}$  in a  $[100]$  Magnetic Field: Y. Shimura, Y. Ohta, T. Sakakibara, A. Sakai and S. Nakatsuji, *J. Phys. Soc. Jpn.* **82** (2013) 043705(1-4).
4.  $^\dagger^*$  High-Field Phase Diagram of  $\text{SmRu}_4\text{P}_{12}$  Determined by Ultrasonic Measurements in Pulsed Magnetic Field up to 55 T: M. Yoshizawa, H. Mitamura, F. Shichinomiya, S. Fukuda, Y. Nakanishi, H. Sugawara, T. Sakakibara and K. Kindo, *J. Phys. Soc. Jpn.* **82** (2013) 033602(1-5).

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\* Joint research among groups within ISSP.

5. Verification of Anisotropic *s*-Wave Superconducting Gap Structure in CeRu<sub>2</sub> from Low-Temperature Field-Angle-Resolved Specific Heat Measurements: S. Kittaka, T. Sakakibara, M. Hedo, Y. Onuki and K. Machida, *J. Phys. Soc. Jpn.* **82** (2013) 123706(1-4).
6. †\* Long-range order and spin-liquid states of polycrystalline Tb<sub>2+x</sub>Ti<sub>2-x</sub>O<sub>7+y</sub>: T. Taniguchi, H. Kadowaki, H. Takatsu, B. Fåk, J. Ollivier, T. Yamazaki, T. J. Sato, H. Yoshizawa, Y. Shimura, T. Sakakibara, T. Hong, K. Goto, L. R. Yaraskavitch and J. B. Kycia, *Phys. Rev. B* **87** (2013) 060408R(1-5).
7. †\* Quasi-one-dimensional S=1/2 Heisenberg antiferromagnetic chain consisting of the organic radical p-Br-V: K. Iwase, H. Yamaguchi, T. Ono, Y. Hosokoshi, T. Shimokawa, Y. Kono, S. Kittaka, T. Sakakibara, A. Matsuo and K. Kindo, *Phys. Rev. B* **88** (2013) 184431(1-5).
8. †\* Various regimes of quantum behavior in an S=1/2 Heisenberg antiferromagnetic chain with fourfold periodicity: H. Yamaguchi, T. Okubo, K. Iwase, T. Ono, Y. Kono, S. Kittaka, T. Sakakibara, A. Matsuo, K. Kindo and Y. Hosokoshi, *Phys. Rev. B* **88** (2013) 174410(1-5).
9. Determining the Surface-To-Bulk Progression in the Normal-State Electronic Structure of Sr<sub>2</sub>RuO<sub>4</sub> by Angle-Resolved Photoemission and Density Functional Theory: C. N. Veenstra, Z. -H. Zhu, B. Ludbrook, M. Capsoni, G. Levy, A. Nicolaou, J. A. Rosen, R. Comin, S. Kittaka, Y. Maeno, I. S. Elfimov and A. Damascelli, *Phys. Rev. Lett.* **110** (2013) 097004(1-5).
10. † Unconventional Magnetic and Thermodynamic Properties of S=1/2 Spin Ladder with Ferromagnetic Legs: H. Yamaguchi, K. Iwase, T. Ono, T. Shimokawa, H. Nakano, Y. Shimura, N. Kase, S. Kittaka, T. Sakakibara, T. Kawakami and Y. Hosokoshi, *Phys. Rev. Lett.* **110** (2013) 157205(1-5).
11. 高次多極子をもたらす磁場誘起相：志村 恭通，榊原 俊郎，大貫 惇睦，*固体物理* **48** (2013) 721-727.
12. Magnetization steps in Yb<sub>2</sub>Pt<sub>2</sub>Pb with the Shastry-Sutherland lattice: Y. Shimura, T. Sakakibara, K. Iwakawa, Y. Onuki and K. Sugiyama, *J. Kor. Phys. Soc.* **63** (2013) 551-554.
13. Singlet-triplet crossover in the two-dimensional dimer spin system YbAl<sub>3</sub>C<sub>3</sub>: S. Kittaka, T. Sugiyama, Y. Shimura, T. Sakakibara, S. Matsuda and A. Ochiai, *J. Kor. Phys. Soc.* **62** (2013) 2088-2092.
14. † Fine-Tuning of Magnetic Interactions in Organic Spin Ladders: H. Yamaguchi, H. Miyagai, T. Shimokawa, K. Iwase, T. Ono, Y. Kono, N. Kase, K. Araki, S. Kittaka, T. Sakakibara, T. Kawakami, K. Okunishi and Y. Hosokoshi, *J. Phys. Soc. Jpn.* **83** (2014) 033707(1-4).
15. Novel Electronic States of Heavy Fermion Compound YbCo<sub>2</sub>Zn<sub>20</sub>: F. Honda, Y. Taga, Y. Hirose, S. Yoshiuchi, Y. Tomooka, M. Ohya, J. Sakaguchi, T. Takeuchi, R. Settai, Y. Shimura, T. Sakakibara, I. Sheikin, T. Tanaka, Y. Kubo and Y. Onuki, *J. Phys. Soc. Jpn.* **83** (2014) 044703(1-9).
16. † Possible Evolution of Antiferromagnetism in Zn-Doped Heavy-Fermion Superconductor CeCoIn<sub>5</sub>: M. Yokoyama, K. Fujimura, S. Ishikawa, M. Kimura, T. Hasegawa, I. Kawasaki, K. Tenya, Y. Kono and T. Sakakibara, *J. Phys. Soc. Jpn.* **83** (2014) 033706(1-5).
17. Thermodynamic Study of Nodal Structure and Multiband Superconductivity of KFe<sub>2</sub>As<sub>2</sub>: S. Kittaka, Y. Aoki, N. Kase, T. Sakakibara, T. Saito, H. Fukazawa, Y. Kohori, K. Kihou, C. Ho Lee, A. Iyo, H. Eisaki, K. Deguchi, N. K. Sato, Y. Tsutsumi and K. Machida, *J. Phys. Soc. Jpn.* **83** (2014) 013704(1-4).
18. †\* Field-induced incommensurate phase in the strong-rung spin ladder with ferromagnetic legs: H. Yamaguchi, H. Miyagai, M. Yoshida, M. Takigawa, K. Iwase, T. Ono, N. Kase, K. Araki, S. Kittaka, T. Sakakibara, T. Shimokawa, T. Okubo, K. Okunishi, A. Matsuo and Y. Hosokoshi, *Phys. Rev. B* **89** (2014) 220402.
19. Measurement of the spin-orbit coupling in superconducting Sr<sub>2</sub>RuO<sub>4</sub> using polarized light and spin-resolved photoemission spectroscopy: Evidence for a breakdown in the singlets and triplets pairing mechanisms: C. N. Veenstra, Z. -H. Zhu, M. Raichle, B. M. Ludbrook, A. Nicolaou, B. Slomski, G. Landolt, S. Kittaka, Y. Maeno, J. H. Dil, I. S. Elfimov, M. W. Haverkort and A. Damascelli, *Phys. Rev. Lett.* **112** (2014) 127002(1-4).
20. Multiband superconductivity with unexpected deficiency of nodal quasiparticles in CeCu<sub>2</sub>Si<sub>2</sub>: S. Kittaka, Y. Aoki, Y. Shimura, T. Sakakibara, S. Seiro, C. Geibel, F. Steglich, H. Ikeda and K. Machida, *Phys. Rev. Lett.* **112** (2014) 067002(1-5).
21. \* Magnetization and Specific Heat of the Caged Compound PrV<sub>2</sub>Al<sub>20</sub>: K. Araki, Y. Shimura, N. Kase, T. Sakakibara, A. Sakai and S. Nakatsuji, *J. Phys. Soc. Jpn.* (2014), in print.

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† Joint research with outside partners.

## Mori group

We have successfully developed and characterized the functional molecular materials. The major achievements in 2013 are (1) to discover the novel spin liquid state of purely organic single-component crystal  $\kappa\text{-H}_3(\text{Cat-EDT-TTF})_2$ , (2) to develop the proton-electron coupled molecular conductor with tuning  $\pi$ -electron bandwidth and hydrogen bond, and (3) to clarify the electronic state between 3/4-filled and effective 1/2-filled band structure by optical measurement for pressure-induced superconductor  $\beta$ -(*meso*-DMBEDT-TTF) $_2\text{PF}_6$ .

1. Optical Conductivity Measurement of a Dimer Mott-Insulator to Charge-Order Phase Transition in a Two-Dimensional Quarter-Filled Organic Salt Compound: R. Okazaki, Y. Ikemoto, T. Moriwaki, T. Shikama, K. Takahashi, H. Mori, H. Nakaya, T. Sasaki, Y. Yasui and I. Terasaki, *Phys. Rev. Lett.* **111** (2013) 217801.
2. †Fabrication of a field effect transistor structure using charge-ordered organic materials  $\alpha$ -(BEDT-TTF) $_2\text{I}_3$  and  $\alpha'$ -(BEDT-TTF) $_2\text{IBr}_2$ : M. Kimata, T. Ishihara, A. Ueda, H. Mori and H. Tajima, *Synth. Met.* **173** (2013) 43-45.
3. Pyridone derivatives carrying radical moieties: Hydrogen-bonded structures, magnetic properties, and metal coordination: M. Ueda, T. Mochida and H. Mori, *Polyhedron* **52** (2013) 755-760.
4. Crystal Architectures and Magnetic Properties of Alkylferrocenium Salts with  $F_n\text{TCNQ}(n = 0, 2, 4)$ : Effect of Substituents on the Self-Assembled Structures: T. Mochida, T. Akasaka, Y. Funasako, Y. Nishio and H. Mori, *Crystal Growth & Design* **13** (2013) 4460.
5. Hydrogen bond-promoted metallic state in a purely organic single-component conductor under pressure: T. Isono, H. Kamo, A. Ueda, K. Takahashi, A. Nakao, R. Kumai, H. Nakao, K. Kobayashi, Y. Murakami and H. Mori, *Nat. Commun.* **4** (2013) 1344-1349.
6. Gapless Quantum Spin Liquid in an Organic Spin-1/2 Triangular-Lattice  $\kappa\text{-H}_3(\text{Cat-EDT-TTF})_2$ : T. Isono, H. Kamo, A. Ueda, K. Takahashi, M. Kimata, H. Tajima, S. Tsuchiya, T. Terashima, S. Uji and H. Mori, *Phys. Rev. Lett.* **112** (2014) 177201.
7. Biferrocenium salts with magnetite-like mixed-valence iron: coexistence of  $\text{Fe}^{3+}$  and  $\text{Fe}^{2.5+}$  in the crystal: T. Mochida, E. Nagabuchi, M. Takahashi and H. Mori, *Chem. Commun.* **50** (2014) 2481.
8. Protonation of Pyridyl-Substituted TTF Derivatives: Substituent Effects in Solution and in the Proton-Electron Correlated Charge-Transfer Complexes: S. C. Lee, A. Ueda, A. Nakao, R. Kumai, H. Nakao, Y. Murakami and H. Mori, *Chem. Eur. J.* **20** (2014) 1909.
9. Charge-Transfer Salts of Biferrocene Derivatives with  $F_2^-$  and  $F_4^-$ -Tetracyanoquinodimethane: Correlation Between Donor-Acceptor Ratios and Cation Valence States: T. Mochida, Y. Funasako, E. Nagabuchi and H. Mori, *Crystal Growth & Design* **14** (2014) 1459.
10. Synergistic Spin Transition between Spin Crossover and Spin-Peierls-like Singlet Formation in the Halogen-Bonded Molecular Hybrid System:  $[\text{Fe}(\text{Iqsal})_2][\text{Ni}(\text{dmit})_2]\cdot\text{CH}_3\text{CN}\cdot\text{H}_2\text{O}$ : K. Fukuroi, K. Takahashi, T. Mochida, T. Sakurai, H. Ohta, T. Yamamoto, Y. Einaga and H. Mori, *Angew. Chem. Int. Ed.* **53** (2014) 1983.
11. 単成分純有機金属材料で金属伝導は可能か?: 森 初果, 上田 顕, *化学* **68** (2013) 64-65.
12. 磁性と伝導性が相関した多重機能性分子性物質の開発: 森 初果, 高橋 一志, *まぐね* **8** (2013) 148-154.
13. はたらくこと 生きること理工系女性の想い: 森 初果, *日刊工業新聞* (2013).
14. 化学の力を生かした新しい分子性機能材料の開発: 森 初果, *化学* **69**, No1 (2014) 20-21.
15. 金属状態を示す純有機単成分導体: 森 初果, *工業材料* **62** No1 (2014) 26-27.

## Nakatsuji group

Our group explores novel quantum phases and phase transitions in rare-earth and transition metal based compounds. The followings are some relevant results obtained in 2013. (1) We have found that the metallic spin ice compound  $\text{Pr}_2\text{Ir}_2\text{O}_7$  exhibits quantum criticality in a nontrivial semimetallic state. (2) The Fe doping at the Al site in  $\alpha\text{-YbAlB}_4$  induces an antiferromagnetic ordering whose ordering temperature goes up to 10 K, which is the highest among the Yb based heavy fermion materials. The large enhancement of the magnetic ordering indicates that the mixed valence plays an important role. (3) Finally, our success in synthesizing high quality single crystals of  $\text{PrTr}_2\text{Al}_{20}$  allows us to reveal that the superconductivity in  $\text{PrTi}_2\text{Al}_{20}$  and the antiferro-quadrupolar transition in  $\text{PrV}_2\text{Al}_{20}$  can be easily suppressed by disorder. This highlights the importance of high quality crystals for the study of strong hybridization effects in quadrupolar Kondo systems.

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\* Joint research among groups within ISSP.

1. Conduction electron spin resonance in  $\text{AlB}_2$ : L. M. Holanda, L. Mendonça-Ferreira, R. A. Ribeiro, J. M. Osorio-Guillén, G. M. Dalpian, K. Kuga, S. Nakatsuji, Z. Fisk, R. R. Urbano, P. G. Pagliuso and C. Rettori, *J. Phys.: Condens. Matter* **25** (2013) 216001.
2. \* Evidence of a High-Field Phase in  $\text{PrV}_2\text{Al}_{20}$  in a [100] Magnetic Field: Y. Shimura, Y. Ohta, T. Sakakibara, A. Sakai and S. Nakatsuji, *J. Phys. Soc. Jpn.* **82** (2013) 043705(1-4).
3. Determination of long-range all-in-all-out ordering of  $\text{Ir}^{4+}$  moments in a pyrochlore iridate  $\text{Eu}_2\text{Ir}_2\text{O}_7$  by resonant x-ray diffraction: H. Sagayama, D. Uematsu, T. Arima, K. Sugimoto, J. J. Ishikawa, E. O'Farrell and S. Nakatsuji, *Phys. Rev. B* **87** (2013) 100403(4 pages).
4. Magnetic excitations and c-f hybridization effect in  $\text{PrTi}_2\text{Al}_{20}$  and  $\text{PrV}_2\text{Al}_{20}$ : Y. Tokunaga, H. Sakai, S. Kambe, A. Sakai, S. Nakatsuji and H. Harima, *Phys. Rev. B* **88** (2013) 085124.
5. Dynamical spin-orbital correlation in the frustrated magnet  $\text{Ba}_3\text{CuSb}_2\text{O}_9$ : Y. Ishiguro, K. Kimura, S. Nakatsuji, S. Tsutsui, A. Q. R. Baron, T. Kimura and Y. Wakabayashi, *Nat. Commun.* **4** (2013) 2022(1-6).
6. Quantum fluctuations in spin-ice-like  $\text{Pr}_2\text{Zr}_2\text{O}_7$ : K. Kimura, S. Nakatsuji, J.-J. Wen, C. Broholm, M. B. Stone, E. Nishibori and H. Sawa, *Nat. Commun.* **4** (2013) 1934(1-6).
7. \* Chemical effects of high-resolution Yb  $L_{\gamma 4}$  emission spectra: a possible probe for chemical analysis: H. Hayashi, N. Kanai, N. Kawamura, Y. H. Matsuda, K. Kuga, S. Nakatsuji, T. Yamashita and S. Ohara, *X-Ray Spectrom.* **42** (2013) 450-455.
8. Low temperature transport properties of the quadrupolar Kondo lattice system  $\text{PrTi}_2\text{Al}_{20}$ : A. Sakai and S. Nakatsuji, *J. Kor. Phys. Soc.* **63** (2013) 398-400.
9. Magnetic order induced by Fe doping in the intermediate valence system  $\beta\text{-YbAlB}_4$ : K. Kuga and S. Nakatsuji, *J. Kor. Phys. Soc.* **63** (2013) 549-550.
10. Mössbauer spectroscopy of Fe-doped valence-fluctuating  $\alpha\text{-YbAlB}_4$ : Y. Sakaguchi, S. Ikeda, H. Kobayashi, K. Kuga, K. Sone and S. Nakatsuji, *J. Kor. Phys. Soc.* **62** (2013) 2146-2149.
11. Single-crystal study on the low-temperature magnetism of the pyrochlore magnet  $\text{Pr}_2\text{Zr}_2\text{O}_7$ : K. Kimura, S. Nakatsuji and A. A. Nugroho, *J. Kor. Phys. Soc.* **63** (2013) 719-721.
12. \* Synchrotron X-ray spectroscopy study on the valence state in  $\alpha$ - and  $\beta$ - $\text{YbAlB}_4$  at low temperatures and high magnetic fields: Y. H. Matsuda, T. Nakamura, K. Kuga, S. Nakatsuji, S. Michimura, T. Inami, N. Kawamura and M. Mizumaki, *J. Kor. Phys. Soc.* **62** (2013) 1778-1781.
13. Quantum criticality in a metallic spin liquid: Y. Tokiwa, J. J. Ishikawa, S. Nakatsuji and P. Gegenwart, *Nature Mater.* **13** (2014) 356.
14. X-ray Photoemission and X-ray Absorption Spectroscopy of Hexagonal  $\text{Ba}_3\text{CuSb}_2\text{O}_9$ : T. Sugimoto, T. Mizokawa, H. Wadati, K. Takubo, A. Damascelli, T. Z. Regier, G. A. Sawatzky, N. Katayama, H. Sawa, K. Kimura and S. Nakatsuji, *J. Kor. Phys. Soc.* **63** (2014) 549-550.
15. \* Heavy fermion superconductivity under pressure in the quadrupole system  $\text{PrTi}_2\text{Al}_{20}$ : K. Matsubayashi, T. Tanaka, J. Suzuki, A. Sakai, S. Nakatsuji, K. Kitagawa, Y. Kubo and Y. Uwatoko, *J. Phys. Soc. Jpn.* (2014), in print.
16. Magnetic and Thermal Properties of the Single Crystalline  $\text{Pr}_2\text{Zr}_2\text{O}_7$  in a [111] field: K. Kimura and S. Nakatsuji, *J. Phys. Soc. Jpn.* (2014), in print.
17. \* Magnetization and Specific Heat of the Caged Compound  $\text{PrV}_2\text{Al}_{20}$ : K. Araki, Y. Shimura, N. Kase, T. Sakakibara, A. Sakai and S. Nakatsuji, *J. Phys. Soc. Jpn.* (2014), in print.
18. \* Magnetization of Yb-based mixed-valent compounds at megagauss fields: T. Terashima, Y. H. Matsuda, K. Kuga, Y. Matsumoto and S. Nakatsuji, *J. Phys. Soc. Jpn.* (2014), in print.
19. Sample Dependence of the Quadrupolar Transition in the Nonmagnetic cubic  $\Gamma_3$  Compound  $\text{PrV}_2\text{Al}_{20}$ : M. Tsujimoto, A. Sakai and S. Nakatsuji, *J. Phys. Soc. Jpn.* (2014), in print.
20. Structural and Magnetic Properties of  $\alpha\text{-Yb}(\text{Al}_{1-x}\text{Fe}_x)\text{B}_4$  under Hydrostatic Pressure: Y. Sakaguchi, S. Ikeda, K. Kuga, S. Nakatsuji, N. Hirao, Y. Ohishi and H. Kobayashi, *J. Phys. Soc. Jpn.* (2014), in print.
21. Superconducting properties of the ferroquadrupolar cubic  $\Gamma_3$  compound  $\text{PrTi}_2\text{Al}_{20}$ : A. Sakai, K. Kuga and S. Nakatsuji, *J. Phys. Soc. Jpn.* (2014), in print.

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† Joint research with outside partners.

22. Suppression of the Heavy Fermion State in Magnetic Fields in the Mixed Valent  $\alpha$ -YbAlB<sub>4</sub>: Y. Matsumoto, K. Kentaro and S. Nakatsuji, *J. Phys. Soc. Jpn.* (2014), in print.
23. Two magnetic phases in  $\alpha$ -YbAl<sub>1-x</sub>Fe<sub>x</sub>B<sub>4</sub>: K. Kuga, S. Suzuki and S. Nakatsuji, *J. Phys. Soc. Jpn.* (2014), in print.
24. 銅酸化物における乱れに強い量子液体状態：中辻 知，澤 博，「超伝導現象と高温超伝導体」，新日本編集企画，(NTS 出版社，2013)，475-481.

## Ohgushi group

Our group is focused on an exploratory synthesis and characterization of oxides, chalcogenides, and intermetallics. The major achievements in the fiscal year 2013 are (1) finding of new superconductivity in anti-post-perovskite compounds, and (2) elucidation of orbital states of iridium oxides by means of resonant x-ray diffraction.

1. \* Observation of Phonon-Assisted Magnon Absorption in Spin-Orbit Coupling Induced Mott Insulator Sr<sub>2</sub>IrO<sub>4</sub>: Y. Hirata, H. Tajima and K. Ohgushi, *J. Phys. Soc. Jpn.* **82** (2013) 035002(1-2).
2. Complex orbital state stabilized by strong spin-orbit coupling in a metallic iridium oxide IrO<sub>2</sub>: Y. Hirata, K. Ohgushi, J.-I. Yamaura, H. Ohsumi, S. Takeshita, M. Takata and T. Arima, *Phys. Rev. B* **87** (2013) 161111(1-5).
3. Magnetoelasticity in ACr<sub>2</sub>O<sub>4</sub> spinel oxides (A = Mn, Fe, Co, Ni, and Cu): V. Kocsis, S. Bordács, D. Varjas, K. Penc, A. Abouelsayed, C. A. Kuntscher, K. Ohgushi, Y. Tokura and I. Kézsmárki, *Phys. Rev. B* **87** (2013) 064416(1-9).
4. \* Mechanism of Enhanced Optical Second-Harmonic Generation in the Conducting Pyrochlore-Type Pb<sub>2</sub>Ir<sub>2</sub>O<sub>7-x</sub> Oxide Compound: Y. Hirata, M. Nakajima, Y. Nomura, H. Tajima, Y. Matsushita, K. Asoh, Y. Kiuchi, A. G. Eguluz, R. Arita, T. Suemoto and K. Ohgushi, *Phys. Rev. Lett.* **110** (2013) 187402(1-5).
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## Division of Condensed Matter Theory

### K. Ueda group

When a simple lattice is depleted in a periodic manner, electronic states of a tight binding model on such a depleted lattice sometimes shows a peculiar feature like a flat band or a Dirac cone. A typical example is the triangular lattice: the honeycomb lattice is obtained by the one third depletion and the kagome lattice by the one quarter depletion. In 2013, we concentrated on the quantum phase transitions of the Hubbard model on the one fifth depleted square lattice. This structure exists in nature in  $\text{CaV}_4\text{O}_9$  and in some iron pnictide compound. At quarter filling the Dirac cone at the gamma point coincides with the Fermi energy and furthermore the Dirac cone touches with an almost flat band forming an  $\text{SU}(3)$  multiplet. We have shown that quantum phase transitions around the symmetric point is controlled by the  $\text{SU}(3)$  Dirac electrons. At half filling the effective theory in the strong coupling limit is a Heisenberg model which shows quantum phase transitions from the dimer singlet to the antiferromagnetic phase and further onto the plaquette singlet phase. Quantum phase transitions of the Hubbard model on this lattice have been investigated by using the cluster dynamical mean field theory.

1.  $\text{SU}(3)$  Dirac Electrons in the 1/5-Depleted Square-Lattice Hubbard Model at 1/4-Filling: Y. Yamashita, M. Tomura, Y. Yanagi and K. Ueda, *Phys. Rev. B* **88** (2013) 195104(1-7).

### Takada group

Employing several techniques including the Green's-function approach, the density-matrix renormalization group, quantum Monte Carlo simulations, band-structure calculations, and several types of variational approaches, we are studying various aspects of quantum many-body problems in condensed matter physics, based mainly on the first-principles Hamiltonian. This year we have studied the following issues: (1) In order to better reproduce the electron-density profile obtained by the diffusion Monte Carlo method for the system of a single atom embedded in the electron gas with arbitrary densities, we have improved on the GGA-PBE version of the exchange-correlation energy functional in the density functional theory. In making this improvement, we have paid special attention to fulfilling the cusp theorem at the atom site. The improved functional will be applied to a wide range of topics in the future, including the phase diagram of the solid hydrogen under high pressures. (2) A further analysis is made for an electron-like elementary excitation (pseudoelectron) in the Luttinger liquid in competition with the spinon and holon excitations by using the powerful self-consistent numerical GWT scheme. (3) Mechanisms of superconductivity are considered in the low-density system in the framework of the  $kp$  perturbation theory with application to the n-type doped  $\text{SrTiO}_3$ . We have considered the effects of various issues such as the ferroelectric soft-phonon exchange, the plasmon contribution, the band multiplicity and the spin-orbit interaction.

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### Oshikawa group

We studied a wide range of fundamental problems in condensed matter theory and statistical mechanics. In particular, we investigated the effects of quantum particle statistics on the ground-state energy. In the case of free particles, a ground state of bosons is given by a Bose-Einstein Condensation of all the particles into the lowest-energy single-particle state. In contrast, the ground

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† Joint research with outside partners.

state of fermions is given by putting the particles to lowest-energy single-particle state, but with the restriction that no more than one particle can occupy an identical state (Pauli exclusion principle). Thus the ground-state energy for the identical Hamiltonian would be higher in the case of fermions, compared to the case of bosons. However, the comparison becomes not trivial when the particles are interacting. In fact, we established several examples in which the hard-core bosons have a higher ground-state energy than the corresponding fermions. We have also provided a novel understanding how the particle statistics affects the ground-state energy: Fermi statistics introduces a sort of frustration among hoppings of many particles. When there is no other frustration among hoppings, we proved that the bosons have a lower ground-state energy than the corresponding fermions, even in the presence of interactions. On the other hand, when frustration is introduced through phases of hopping amplitudes, the effects may partially cancel with each other, resulting in a reversal of the ground-state energy.

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2. <sup>†</sup>Electron spin resonance shifts in S=1 antiferromagnetic chains: S. C. Furuya, Y. Maeda and M. Oshikawa, *Phys. Rev. B* **87** (2013) 125122 (1-10).
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4. <sup>†</sup>Hole statistics and superfluid phases in quantum dimer models: C. A. Lamas, A. Ralko, M. Oshikawa, D. Poilblanc and P. Pujol, *Phys. Rev. B* **87** (2013) 104512(1-20).
5. <sup>†</sup>Response to a twist in systems with  $Z_p$  symmetry: The two-dimensional p-state clock model: Y. Kumano, K. Hukushima, Y. Tomita and M. Oshikawa, *Phys. Rev. B* **88** (2013) 104427 (1-6).
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7. <sup>†</sup>Quantum criticality in an asymmetric three-leg spin tube: A strong rung-coupling perspective: Y. Fuji, S. Nishimoto, H. Nakada and M. Oshikawa, *Phys. Rev. B* **89** (2014) 054425 (1-13).
8. <sup>†</sup>Valence bond distribution and correlation in bipartite Heisenberg antiferromagnets: D. Schwandt, F. Alet and M. Oshikawa, *Phys. Rev. B* **89** (2014) 104416 (1-14).

## Tsunetsugu group

We have investigated novel phases of non-Kramers doublets realized in the heavy fermion compound  $\text{PrIr}_2\text{Zn}_{20}$  and related materials. Non-Kramers doublet is a ground state of  $f^2$  electron configuration protected by cubic symmetry of the crystalline field. Based on a microscopic model and an effective field theory, we have used symmetry arguments and mean-field approach to study possible symmetry breaking at low temperatures with and without magnetic field. We have found various antiferro quadrupole ordered phases depending on the magnetic field direction. The most important ingredient is the presence of a unique  $Z_3$  anisotropy in the order parameter space, and in particular, the zero-field order corresponds to the spontaneous breaking of  $Z_3 \times Z_2$  symmetry. This also results in unusual divergence of quadrupole susceptibility in several channels near the critical point. This may be related to observed singularity in ultrasound measurements. We have also numerically studied doublon dynamics near the Mott metal-insulator transition. It has been long believed that the Mott transition is a binding-unbinding transition of doublons and holons, but this point has been directly examined only by equal-time correlations. We have performed large-scale computations of cluster dynamical mean-field theory for the half-filled Hubbard model on the triangular lattice, and calculated dynamical correlations of doublons and holons on the same site and also between nearest-neighbor sites. The results show drastic changes in their dynamics between the metallic and insulating phases. In particular, the doublon-holon pair correlation shows fluctuations up to a very long time in the metallic phase, while the correlation decays very quickly in the insulating phase. This supports the binding-unbinding transition picture of the Mott transition. (Reference: Toshihiro Sato and Hirokazu Tsunetsugu, arXiv:1404.6598) Quantum impurities coupled to Tomonaga-Luttinger liquids are interesting physical systems including an impurity in quantum wire, a spin coupled to a two-dimensional topological insulator etc. We have developed a new method of quantum Monte Carlo simulation with continuous time formulation. This is based on the duality between electrons and bosons, and this results in the advantage of negative sign free nature. The new method is applied to various problems and scaling properties of correlation functions are examined. (Reference: K. Hattori and A. Rosch, arXiv: 1405.3300)

1. Continuous-Time Quantum Monte Carlo Approach for Impurity Anderson Models with Phonon-Assisted Hybridizations: K. Hattori, *J. Phys. Soc. Jpn.* **82** (2013) 064709 (5 pages).
2. Exotic disordered phases in the quantum J1-J2 model on the honeycomb lattice: H. Zhang and C. A. Lamas, *Phys. Rev. B* **87** (2013) 024415 (10 pages).
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\* Joint research among groups within ISSP.

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### Kohmoto group

Energy versus magnetic field (Hofstadter butterfly diagram) in twisted bilayer graphene is studied theoretically. If we take the usual Landau gauge, we cannot take a finite periodicity even when the magnetic flux through a supercell is a rational number. We show that the periodic Landau gauge, which has the periodicity in one direction, makes it possible to obtain the Hofstadter butterfly diagram. Since a supercell can be large, magnetic flux through a supercell normalized by the flux quantum can be a fractional number with a small denominator, even when a magnetic field is not extremely strong. As a result, quantized Hall conductance can be a solution of the Diophantine equation which cannot be obtained by the approximation of the linearized energy dispersion near the Dirac points.

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2. †The Spectral Shift Function and the Friedel Sum Rule: M. Kohmoto, T. Koma and S. Nakamura, *Ann. Henri Poincaré* **14** (2013) 1413-1424.

### Sugino group

We have advanced the first-principles molecular dynamics approach to the electrochemical interfaces. This was done by improving the effective screening medium (ESM) method. With the method, new results were obtained regarding the planar and particle catalysts and the mechanism of the reactions. We have continued to develop a many-body Green's function approach to the spectroscopy and began to obtain promising results. Progress has been made on the tensor network approach to obtain accurate density matrix of molecules.

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### Kato group

The main research subject in our laboratory is theory of nonequilibrium properties in nanoscale devices. We have performed (1) evaluation of coherence in single-photon and single-electron generation quantum, (2) exact calculation of transport properties in the Anderson impurity at high bias voltages, and (3) Kondo-like phenomena in heat transport through a local two-state system.

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† Joint research with outside partners.



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4. \* Experimental Verification of Comparability between Spin-Orbit and Spin-Diffusion Lengths: Y. Niimi, D. Wei, H. Idzuchi, T. Wakamura, T. Kato and Y. Otani, *Phys. Rev. Lett.* **110** (2013) 016805.
5. Kondo Signature in Heat Transfer via a Local Two-State System: K. Saito and T. Kato, *Phys. Rev. Lett.* **111** (2013) 214301(1-5).
6.  $1/(N-1)$  expansion approach to full-counting statistics for the SU(N) Anderson model: A. Oguri and R. Sakano, *J. Kor. Phys. Soc.* **63** (2013) 423-427.
7. Dephasing in single-electron generation due to environmental noise probed by Hong-Ou-Mandel interferometry: E. Iyoda, T. Kato, K. Koshino and T. Martin, *Phys. Rev. B* **89** (2014) 205318(1-8).
8. メゾスコピック系の物理—基礎から最近の話題まで—(第 58 回物性若手夏の学校: 講義): 加藤 岳生, 物性研究・電子版 **3** (2014) 031201(1-26).

## Division of Nanoscale Science

### Iye group

Thermoelectric effect and high frequency conduction in GaAs/AlGaAs 2DEG subjected to periodic potential modulation (lateral superlattice) has been investigated. Commensurability oscillation in thermoelectric power is observed in one-dimensional lateral superlattice sample. AC conductivity in the quantum Hall plateau region of a hexagonal lateral superlattice sample exhibits a few characteristic resonance peaks.

1. \* Control of magnetic anisotropy in (Ga,Mn)As with etching depth of specimen boundaries: Y. Hashimoto, Y. Iye and S. Katsumoto, *J. Cryst. Growth* **378** (2013) 381.
2. \* Suppression of Andreev current due to transverse current flow in an InAs two-dimensional electrons: Y. Takahashi, Y. Hashimoto, Y. Iye and S. Katsumoto, *J. Cryst. Growth* **378** (2013) 400.
3. \* Spin Hall reduction of Josephson effect in InAs two-dimensional electrons: T. Nakamura, Y. Takahashi, Y. Hashimoto, D. H. Yun, S. W. Kim, Y. Iye and S. Katsumoto, *Phys. Status Solidi C* **10** (2013) 1473.
4. Commensurability oscillations in the rf conductivity of unidirectional lateral superlattices: measurement of anisotropic conductivity by coplanar waveguide: A. Endo, T. Kajioka and Y. Iye, *J. Phys. Soc. Jpn* **82** (2013) 054710(1-7).
5. Diffusion Thermopower of Quantum Hall States Measured in Corbino Geometry: S. Kobayakawa, A. Endo and Y. Iye, *J. Phys. Soc. Jpn* **82** (2013) 053702(1-4).
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### Katsumoto group

The two-electron tunneling process to a side-coupled quantum dot has been applied to detect spin polarization in the target device. The method is most powerful among so far developed and the device voltage dependence can be measured. We have revealed that the polarization mechanism at so called 0.5 plateau is the Stern-Gelach type spin-filter while that at 1.0 plateau is the spin rotation predicted a decade ago.

1. Robustness of spin filtering against current leakage in a Rashba-Dresselhaus-Aharonov-Bohm interferometer: S. Matiyahu, A. Aharony, O. Entin-Wohlman and S. Katsumoto, *Phys. Rev. B* **87** (2013) 205438(1-8).
2. †\* Adiabatic measurements of magneto-caloric effects in pulsed high magnetic fields up to 55 T: T. Kihara, Y. Kohama, Y. Hashimoto, S. Katsumoto and M. Tokunaga, *Rev. Sci. Instrum.* **84** (2013) 074901(1-7).

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\* Joint research among groups within ISSP.

3. \* Control of magnetic anisotropy in (Ga,Mn)As with etching depth of specimen boundaries: Y. Hashimoto, Y. Iye and S. Katsumoto, *J. Cryst. Growth* **378** (2013) 381.
4. \* Suppression of Andreev current due to transverse current flow in an InAs two-dimensional electrons: Y. Takahashi, Y. Hashimoto, Y. Iye and S. Katsumoto, *J. Cryst. Growth* **378** (2013) 400.
5. \* Spin Hall reduction of Josephson effect in InAs two-dimensional electrons: T. Nakamura, Y. Takahashi, Y. Hashimoto, D. H. Yun, S. W. Kim, Y. Iye and S. Katsumoto, *Phys. Status Solidi C* **10** (2013) 1473.
6. \* Heat-pulse measurements of specific heat in 36 ms pulsed magnetic fields: Y. Kohama, Y. Hashimoto, S. Katsumoto, M. Tokunaga and K. Kindo, *Meas. Sci. Technol.* **24** (2013) 115005(1-9).
7. Effect of transverse current on Andreev bound state: Y. Takahashi, Y. Hashimoto, D. H. Yun, S. W. Kim, T. Nakamura, Y. Iye and S. Katsumoto, in: *AIP Conference Proceedings, "International Conference on Physics of Semiconductors"*, edited by T. Ihn (AIP, 2013), 345.
8. \* Mechanical modification of magnetic anisotropy in (Ga,Mn)As: Y. Hashimoto, Y. Iye and S. Katsumoto, in: *AIP Conference Proceedings "International Conference on Physics of Semiconductors"*, edited by T. Ihn (AIP, 2013), 347.
9. 量子の匠：勝本 信吾，(丸善，東京，2014).

## Otani group

We have studied on three topics including spin Hall effect, spin diffusion length, and magnonic crystals. Firstly we have applied our non-local spin injection technique to 5d iridium oxide, and succeeded in detecting a very large inverse spin Hall resistivity at room temperature which guarantees this material as a good spin current detector. Secondly we experimentally confirmed that weak antilocalization measurements can be employed as a complementary method for determining the spin diffusion lengths of noble metals. Thirdly in collaboration with Indian group lead by Prof. Barman in Bose Center Kolkata, we have performed all-optical time-resolved magneto-optical Kerr microscope measurements and found that the anisotropic propagation of spin waves are tunable by arranging different symmetries in the form of artificial ferromagnetic nanodot lattices. The observations are important for further development in magnonic crystal based devices.

1. \* Experimental Verification of Comparability between Spin-Orbit and Spin-Diffusion Lengths: Y. Niimi, D. Wei, H. Idzuchi, T. Wakamura, T. Kato and Y. Otani, *Phys. Rev. Lett.* **110** (2013) 016805.
2. Configurational anisotropic spin waves in cross-shaped Ni<sub>80</sub>Fe<sub>20</sub> nanoelements: B. K. Mahato, B. Rana, R. Mandal, D. Kumar, S. Barman, Y. Fukuma, Y. Otani and A. Barman, *Appl. Phys. Lett.* **102** (2013) 192402.
3. Impact of interface properties on spin accumulation in dual-injection lateral spin valves: H. Idzuchi, S. Karube, Y. Fukuma, T. Aoki and Y. Otani, *Appl. Phys. Lett.* **103** (2013) 162403.
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8. Effect of anisotropic spin absorption on the Hanle effect in lateral spin valves: H. Idzuchi, Y. Fukuma, S. Takahashi, S. Maekawa and Y. Otani, *Phys. Rev. B* **89** (2014) 081308(R).
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10. Spin Injection into a Superconductor with Strong Spin-Orbit Coupling: T. Wakamura, N. Hasegawa, K. Ohnishi, Y. Niimi and Y. Otani, *Phys. Rev. Lett.* **112** (2014) 036602.

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† Joint research with outside partners.

## Komori group

Electronic structures of Pt-induced nanowires on the Ge(001) surface were studied by ARPES. Two one-dimensional (1D) metallic surface bands are clearly identified at temperatures much lower than its structural transition temperature. This 1D system exhibits neither Peierls instability nor Luttinger liquid behaviors. The elastic-scattering vectors within the topological surface state (TSS) of a topological insulator  $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{1.7}\text{Se}_{1.3}$  were studied using quasiparticle interference patterns measured by STM. The results are compared by the surface band obtained using time-resolved ARPES. The scattering in the TSS is effectively prohibited in a wide angular range of 100-180°.

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## Yoshinobu group

We conducted several research projects in the fiscal year 2013. (1) The adsorption and activation of CO<sub>2</sub> on Cu(997) studied by SR-PES and IRAS. (2) The adsorption and decomposition of formic acid on Cu(111) studied by SR-PES and IRAS. (3) Spectroscopic characterization and transport properties of the Si(111) native oxide surface with tetrafluorotetracyanoquinodimethane. (4) Electronic structure of alufa-sexithiophene ultra thin films grown on passivated Si(001) surfaces.

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### Hasegawa group

We studied the superconducting proximity effect in real space by using low-temperature scanning tunneling microscopy and spectroscopy aiming at the observation of peculiar superconducting states, such as Fulde–Ferrell–Larkin–Ovchinnikov (FFLO) states and odd-frequency superconductivity. So far, we observed the spatial distribution of superconductivity around an interface between Pb islands and a two-dimensional (2D) diffusive normal metal, and found that the surface steps in the 2D normal metal working as a potential barrier exhibit a significant role on the proximity effect; through the real-space mapping of superconductivity in nano-meter spatial resolution, we observed the steps blocking the propagation of the proximity and enhancing it in confined area between the steps and the super/normal interface. The enhancement is explained with reflectionless tunneling, quantum interference phenomenon between the incident electrons and retro-reflected holes formed by the Andreev reflection at the interface. On a 2D surface superconductor, which can be formed by depositing 1 monolayer In or Pb on Si(111) substrate, we also observed Josephson vortices at the step edges, indicating weakened superconductivity there.

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### Lippmaa group

High-temperature growth studies of magnetite Fe<sub>3</sub>O<sub>4</sub> showed that it is possible to fabricate self-organized arrays of strain-free and uniformly oriented nanoscale pyramids. We hope to use such nanopyramid arrays for studying the multiferroic coupling in magnetite. Nanoscale composite materials based on a ferromagnetic spinel, CoFe<sub>2</sub>O<sub>4</sub> and a ferroelectric perovskite, Bi<sub>5</sub>Ti<sub>3</sub>FeO<sub>15</sub> were characterized in collaboration with our joint-use partners. Saturation magnetism and spin dilution was studied in Pr<sub>0.8</sub>Ca<sub>0.2</sub>MnO<sub>3</sub> to develop a suitably weak ferromagnet for use in superconductor - ferromagnet tunnel junctions. Work proceeded on the development of light-element oxide films with the mapping of the growth mechanisms of BeO.

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## Division of Physics in Extreme Conditions

### Uwatoko group

The present antiferromagnetic state  $T_N=7.5$  K of EuBi<sub>3</sub> with the AuCu<sub>3</sub>-type cubic structure is found to be stable under pressures up to 8 GPa, where the Neel temperature increases with increasing pressure, being  $T_N=16.5$  K at 8 GPa. We have studied the effect of pressure on the superconducting transition temperature of YFe<sub>4</sub>P<sub>12</sub> and LaFe<sub>4</sub>P<sub>12</sub> up to 8 GPa through electrical resistivity measurements in a cubic anvil apparatus.  $T_{SC}$  of both compounds increase to 9.3 K and 8.0 K with increasing pressure, but the slopes decrease gradually with increasing pressure, respectively. In contrast, the  $T_{SC}$  of YRu<sub>4</sub>P<sub>12</sub> and LaRu<sub>4</sub>P<sub>12</sub> monotonically decreases with pressure. The distinct pressure dependences of both  $T_{SC}$  cannot be explained solely from a structural point of view. The pressure dependence of the electrical resistivity of BaCo<sub>2</sub>As<sub>2</sub> single crystal as a function of temperature was measured up to 8 GPa. A hybrid-type piston-cylinder pressure cell for the electron spin resonance (ESR) measurement has been developed that the pressure reaches 2.1 GPa. The cylinder of this pressure cell consists of a NiCrAl inner cylinder and a CuBe outer sleeve, and all inner parts are made of zirconium oxide which has good transmittance to the millimeter and submillimeter waves. We have also developed a transmission-type high-field ESR system having two different modulation methods for this pressure cell.

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† Joint research with outside partners.

## Osada group

In an organic Dirac fermion system  $\alpha$ -(BEDT-TTF)<sub>2</sub>I<sub>3</sub>, the  $\nu=0$  quantum Hall state is realized under magnetic fields resulting from the breaking of four-fold (spin and valley) degeneracy of the singular  $n=0$  Landau level. The recent NMR measurement has suggested the possible transition from the quantum Hall ferromagnetic (QHF) phase to the quantum Hall insulator (QHI) phase around 15 T. To check this possibility, we have performed high-field transport measurement up to 31T using the NHMFL at Tallahassee, USA. The interlayer resistance shows the saturating behavior up to high fields, which reflects the surface transport via helical edge state of the QHF phase. We can see no anomaly in the saturating region, especially around 15T. This result means that the QHF state survives up to 31T with no QHF-QHI transition.

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## Yamashita group

As the first year of Yamashita group, we developed a new probe for thermal-Hall measurement which can be used in VTI system with 16 T magnet. With this probe, we successfully started the study of thermal-transport measurement of a kagome material, Volborthite, to find if there is a thermal-Hall effect due to spinons. Developments of the measurement systems for studies under ultra-low temperatures, on the other hand, did not work out due to malfunctions of dilution refrigerators inherited from Ishimoto and Tajima groups.

## Materials Design and Characterization Laboratory

### Hiroi group

Spinodal decomposition is a ubiquitous phenomenon leading to phase separation from a uniform solution. We show that a spinodal decomposition occurs in a unique combination of two rutile compounds of TiO<sub>2</sub> and VO<sub>2</sub>, which are chemically and physically distinguished from each other: TiO<sub>2</sub> is a wide-gap insulator with photo catalytic activities and VO<sub>2</sub> is assumed to be a strongly correlated electron system which exhibits a dramatic metal-insulator transition at 342 K. The spinodal decomposition takes place below 830 K at a critical composition of 34 mol% Ti, generates a unidirectional composition modulation along the c axis with a wavelength of approximately 6 nm, and finally results in the formation of self-assembled lamella structures made up of Ti-rich and V-rich layers stacked alternately with 30-50 nm wavelengths. A metal-insulator transition is not observed in quenched solid solutions with intermediate compositions but emerges in the thin V-rich layers as the result of phase separation. Interestingly, the metal-insulator transition remains as sharp as in pure VO<sub>2</sub> even in such thin layers and takes place at significantly reduced temperatures of 310-340 K, which is probably due to a large misfit strain induced by lattice matching at the coherent interface.

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12. \*Kagome–Triangular Lattice Antiferromagnet NaBa<sub>2</sub>Mn<sub>3</sub>F<sub>11</sub>: H. Ishikawa, T. Okubo, Y. Okamoto and Z. Hiroi, *J. Phys. Soc. Jpn.* **83** (2014) 043703(1-5).

## 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 achievements of 2013 include: (1) clarifying the apparent deconfined critical behavior of the SU(N) J-Q Heisenberg model with a strong corrections to scaling, (2) lattice rotational symmetry breaking in frustrated spin systems, and (3) highly parallelized code for the molecular dynamics simulation of mixed-phase fluid dynamics.

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† Joint research with outside partners.



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## Noguchi group

We have studied the structure formation of surfactant membranes under shear flow. We found that shear can induce a rolled lamellae structure, which structure factor agrees with those of intermediate states during lamellar-to-onion transition measured by time-resolved scattering experiments. We revealed that entropy reduction of membrane fluctuations can induce aggregation of binding proteins in multilamellar membranes. We also studied the effects of anchored polymers on membranes and dynamics of deformable active particles.

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## Materials Synthesis and Characterization group

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\* Joint research among groups within ISSP.

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## Neutron Science Laboratory

### Shibayama group

Shibayama group has been exploring the structure and dynamics of soft matter, especially polymer gels, micelles, and phenolic resin, utilizing a combination of small-angle neutron scattering (SANS), neutron spin echo (NSE), and dynamic light scattering (DLS). The objectives are to elucidate the mysterious relationship between the structure and variety of novel properties/functions of polymer gels/resins. The highlights of 2012 include (1) structural analysis of high performance ion-gel comprising tetra-PEG networks, (2) atomistic molecular dynamics study of cross-linked phenolic resins, (3) rubber elasticity for incomplete polymer networks, (4) kinetic study for AB-type coupling reaction of tetra-arm polymers, (5) optimization of the thickness of a  $\text{ZnS}/(\text{LiF})\text{-Li-6}$  scintillator for a high-resolution detector installed on a focusing small-angle neutron scattering spectrometer (SANS-U), and so on.

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\* Joint research among groups within ISSP.

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### Yoshizawa group

A systematic study on spin dynamics in two-dimensional transition-metal oxides has been carried out with use of the high resolution chopper spectrometer installed at BL12 in the Material and Life Science Facility, J-PARC. In the highly hole-doped region in the layered nickelate, it shows a checkerboard-type spin-charge ordering, and the nature of the excitation spectra changes its character and approaches to the metal-like behavior. Spin fluctuations in several quantum spin systems were also studied.

- <sup>†\*</sup> Long-range order and spin-liquid states of polycrystalline  $Tb_{2+x}Ti_{2-x}O_{7+y}$ : T. Taniguchi, H. Kadowaki, H. Takatsu, B. Fåk, J. Ollivier, T. Yamazaki, T. J. Sato, H. Yoshizawa, Y. Shimura, T. Sakakibara, T. Hong, K. Goto, L. R. Yaraskavitch and J. B. Kycia, *Phys. Rev. B* **87** (2013) 060408R(1-5).
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### 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, there were two important outcomes in the study of ionic liquids. The first one, which was found in the quasielastic neutron scattering (QENS) and viscoelastic measurements, is that the inter-ionic motion is directly associated with the glass transitions in imidazolium-bases ionic liquids. The second one is that the origin of the low- $Q$  diffraction peak, which is a typical property of the ionic liquids, is a local structure similar to that of a liquid-crystalline (SmA) phase. This was obtained from differential scanning calorimetry (DSC) and X-ray diffraction experiments. In the QENS study of a porous coordination polymer MIL-53, we have found that protons are carried by both water and ammonia molecules which are more mobile than those in bulk states. Other than these topics, we have made some progresses in the studies on palladium hydrides and vapor-deposited simple molecular glasses.

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- Heterogeneous Slow Dynamics of Imidazolium Based Ionic Liquids Studied by Neutron Spin Echo: M. Kofu, M. Nagao, T. Ueki, Y. Kitazawa, Y. Nakamura, S. Sawamura, M. Watanabe and O. Yamamuro, *J. Phys. Chem. B* **117** (2013) 2773-2781.
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## Masuda group

Recently the discovery of the multiferroics, i.e., enhanced simultaneous orders in magnetism and dielectricity, revived the study of the magnetoelectric effect. A number of studies had revealed its mechanism and clarified the relationships between dielectric and magnetic structures in homogeneous systems. Next challenge would be to find and study a new magnetoelectric effect in inhomogeneous system. A remarkable example in an inhomogeneous system is a magnet having relaxor property, relaxor magnet. In 2013 our group studied a new relaxor magnet,  $\text{LuFeCoO}_4$ , by combination of bulk properties measurements and neutron diffraction technique. Our study reveals a novel relationship between PNRs and magnetic correlation, and establishes the magnetic and dielectric phase diagrams of the relaxor magnet.

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## International MegaGauss Science Laboratory

### Takeyama group

The electro-magnetic flux compression techniques have been established to generate magnetic fields over 700 T by employing a new type of primary coil (a copper lined iron coil). In such a high magnetic field, a measurement of the magnetic field should be reconsidered. In pulse magnet operation, the magnetic field has been determined by a pick-up coil, wound around a thin rod, converted from the detected induced voltage from  $d\phi/dt$  ( $\phi$ , a magnetic flux), followed by a certain process of calibration. We have found recently that the pick-up coil is not a reliable method anymore in such an extremely high magnetic fields. A Faraday rotation angle of quartz and the other glasses was measured up to a peak field and is calibrated with the signals from the pick-up coil. The present study revealed that the conventional pick-up coil method underestimated the values of the peak fields at least 10 %, so that 730 T ever reported could possibly reach 800 T.

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## Kindo group

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## Tokunaga group

By measuring the resistance of thin-film thermometers deposited on the sample surface, we succeeded in rapid temperature monitoring of the sample with the response time shorter than 0.1 ms. With using this technique, we developed a measurement system of magneto-caloric effects in pulsed high magnetic fields up to 55 T. This technique provides us of novel thermodynamic information of various kind of phase transitions induced in high magnetic fields and also direct information of the entropy in frustrated magnets.

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## Y. Matsuda group

The magnetization process of  $\text{SrCu}_2(\text{BO}_3)_2$  shows exotic multi-plateau structure, indicating the crystallization of the excited triplet dimers with the several fractional fillings in the sea of the singlet dimers. We have succeeded in observing the magnetization curve of  $\text{SrCu}_2(\text{BO}_3)_2$  in ultrahigh magnetic fields of up to 118 Tesla. The long predicted 1/2 plateau has been clearly observed at the field range from 84 to 108 Tesla for the first time. A destructive way of magnetic field generation, single-turn coil method (STC), was used for the experiment. In addition to the magnetization measurement, the cyclotron resonance in ferromagnetic semiconductors and magneto-absorption spectroscopy in solid oxygen have been performed at very high magnetic fields over 100 Tesla. The synchrotron x-ray spectroscopy on Yb-based heavy fermion compounds  $\text{YbRh}_2\text{Si}_2$  and  $\text{YbAlB}_4$  revealed that the valence instability was affected by a strong magnetic field, suggesting the importance of the charge degree of freedom for understanding their exotic properties at very low temperatures.

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## Center of Computational Materials Science

### Akai group

We have developed methodologies that enable us to calculate electronic structure of wide range of systems such as strongly correlated systems and systems in non-equilibrium states. One of them is a scheme of first-principles calculation of the non-equilibrium Green's function of tunnelling junctions in the framework of the Korringa-Kohn-Rostoker (KKR) Green's function method is developed. Another is the optimized effective potential (OEP) method applied to static RPA scheme. The latter includes an elaboration that dissolves a well-known difficulty arising from the indefiniteness inherent in the theory of OEP. One of main topics we are now working on is the theory of permanent magnet. This year we have developed the theory of magnetic anisotropy of Sm-Fe-N magnet, in particular discussing the role of N that experimentally is known to be important to realize the uni-axial magnetic anisotropy of this system.

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### Todo group

We study novel phases and critical phenomena in strongly correlated many-body systems, such as quantum magnets and Bose-Hubbard model, by using the state-of-the-art computational physics techniques like the quantum Monte Carlo method. We also develop new computational algorithms for quantum many-body systems, such as the tensor-network method, study the parallelization technique for supercomputers, and develop open-source software for next-generation parallel simulations: (1) Analysis of quantum phases and quantum phase transitions by local Z<sub>2</sub> Berry phase (2) Critical phenomena of long-range interacting spin model (3) Quantum phase transition of SU(N) J-Q model (4) Irreversible Markov chain Monte Carlo (5) Simulation method for systems with strong spatial anisotropy (6) Parallelization of worm algorithm quantum Monte Carlo method (7) Parallel exact diagonalization package "Rokko".

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## Laser and Synchrotron Research Center

### Suemoto group

To study ultrafast spin dynamics in canted ferromagnets, terahertz pump-Faraday probe experiments were performed on orthoferrites and several new aspects were revealed as follows. (1) Extremely long coherence time and beating phenomena were found in spin precession modes. (2) Dynamics of magnetic anisotropy parameters modified by optical excitation was observed. (3) Resonance enhancement of the spin precession by using a metamaterial structure (split ring resonator) was demonstrated. As for the photoinduced phase transition, femtosecond dynamics in a novel nanocrystalline titanium oxide was studied and ultrafast phase change was confirmed, which guarantees usefulness of this material for optical storage. Newton's ring in soft x-ray region (at 13.9 nm) was firstly observed during the laser ablation process, suggesting an extremely thin and flat expansion front.

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### Shin group

We studied high  $T_c$  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.

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## Takahashi group

We have been studying the structure and phase transition of surfaces and interfaces with diffraction techniques. Topological insulators attract much attention due to potential applications such as spintronics and quantum computing. The structure of a Bi(001)/Bi<sub>2</sub>Te<sub>3</sub>(001) heteroepitaxial film grown on Si(111) was studied with atomic layer resolution by using X-ray crystal truncation rod scattering in combination with a novel structure analysis method. We revealed the Bi thin film is heavily distorted due to the interaction with the substrate Bi<sub>2</sub>Te<sub>3</sub>, resulting in the topological phase transition of the Bi film. We could also get quantitative information on the structural inhomogeneity at the interface between both Bi/Bi<sub>2</sub>Te<sub>3</sub> and Bi<sub>2</sub>Te<sub>3</sub>/Si(111).

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## Akiyama group

In 2013, we started experimental and theoretical study on energy conversion efficiencies and sub-cell internal luminescence yields of tandem solar cells on the basis of a detailed-balance relation. We applied this key relation to the study of intrinsic radiative lifetime of one-dimensional excitons, and fluorescent radiation thermometry at cryogenic temperatures. We also started collaboration on the photoluminescence emission of photoexcited undoped GaAs quantum wells induced by an intense single-cycle terahertz pulse. We intensively studied spectral dynamics in short-pulse generation via gain switching of semiconductor lasers, such as Fabry-Perot GaAs or InGaAs lasers, InGaN VCSELs, and InGaAsP DFB lasers. We developed and characterized double-core-slab-waveguide semiconductor lasers for end optical pumping. We studied the effect of site-directed mutant luciferase on quantitative green and orange/red emission intensities in firefly bioluminescence, and firefly oxyluciferin in enzymatic environment on the basis of stability monitoring. Intensive studies were made with TD-DFT theoretical calculations on electronic states for luciferin and oxyluciferin.

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\* Joint research among groups within ISSP.

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† Joint research with outside partners.

## I. Matsuda group

Developments and experiments of the advanced spectroscopies have been carried out by using vacuum ultraviolet (VUV) and soft X-rays (SX). At SPring-8 BL07LSU, picosecond-time-resolved SX photoemission spectroscopy measurements have been carried out to trace relaxation of photo-excited carriers at metal oxide surfaces. Analyses of the carrier life time have directly revealed the electron-hole recombination process. At Kashiwa campus, dynamics of the Dirac Fermion in a graphene layer is studied by femtosecond-time-resolved VUV photoemission spectroscopy. The transient electron temperature has indicated generation of the cascade carrier multiplication in the femtosecond-time scale. As a part of the undulator development at SPring-8 BL07LSU, phase shifters with electromagnetic coils were mechanically adjusted and installed in the electron storage ring. The phase shifters will be used to make fast polarization switching of the beamline.

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\* Joint research among groups within ISSP.

## Kobayashi group

We have demonstrated a precision spectroscopy in VUV region by using VUV frequency comb.

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## Itatani group

The Itatani group worked mainly on (i) the generation of soft-X-ray high harmonics using a BIBO-based optical parametric chirped pulse amplifier at 1.6  $\mu\text{m}$  and (ii) the generation of intense THz pulses and their application to coherent control of small molecules. Regarding the BIBO-based source, we measured high harmonic spectra up to 330 eV with various experimental parameters such as backing pressures and carrier-envelope phases of the driver pulses. We observed clear CEP-dependences up to the backing pressure of 3 atm, which showed a potential to increase the photon flux of soft-X-ray attosecond pulses. As for the THz generation, we controlled the rotational wavepackets in jet-cooled HBr molecules to achieve molecular orientation (alignment with head-and-tail discrimination). We observed clear signature of molecular orientation by a newly-developed velocity-map imaging apparatus. This is the first clear demonstration of molecular orientation by using intense THz pulses.

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## Harada group

1) Operando soft X-ray RIXS spectroscopy for electronic structure analysis of catalytic reactions: We have developed a novel electrochemical cell system for operando soft X-ray emission spectroscopy for analysis of catalytic reactions. We have applied the system to identify the active site for oxygen reduction reaction in polymer electrolyte fuel cells cathode catalysts. We have observed the electronic structure of iron in an iron phthalocyanine-based cathode catalyst under various working conditions and found that an oxidized iron site exists and is active for oxygen adsorption, which is not expected from ex situ results in which a metallic iron site dominates. 2) Development of the soft X-ray RIXS system around sample manipulation: In order to extend the public use of the soft X-ray emission spectroscopy station we have realized precise temperature control of liquids in the range of  $-5 \sim 80$  °C within  $\pm 1$ K accuracy using an originally developed thermal shielding, and surface cleaning by neutralized ion sputtering and annealing at more than 1000 K by electron bombardment. We also have implemented a liq. He sample cooling system down to 35 K. All these systems are now in operation and open to public. 3) Pioneering work on soft X-ray vibrational RIXS of liquids: Ultrahigh resolution resonant inelastic soft X-ray scattering was applied to observe multiple vibrational excitations in liquid water. By tuning X-ray excitation energy to a particular structure in the X-ray absorption spectrum we have successfully obtained vibrational frequencies well correlate with the OH stretching mode of a particular configuration of water. This enables element- and site-specific vibrational spectroscopy that is not accessible by the conventional IR or Raman spectroscopy.

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† Joint research with outside partners.



1. †\* Selective Probing of the OH or OD Stretch Vibration in Liquid Water Using Resonant Inelastic Soft-X-Ray Scattering: Y. Harada, T. Tokushima, Y. Horikawa, O. Takahashi, H. Niwa, M. Kobayashi, M. Oshima, Y. Senba, H. Ohashi, K.T. Wikfeldt, A. Nilsson, L.G.M. Pettersson and S. Shin, *Phys. Rev. Lett.* **111** (2013) 193001(1-5).
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6. † Unveiling the impurity band induced ferromagnetism in the magnetic semiconductor (Ga,Mn)As: M. Kobayashi, I. Muneta, Y. Takeda, Y. Harada, A. Fujimori, J. Krempaský, T. Schmitt, S. Ohya, M. Tanaka, M. Oshima and V. N. Strocov, *Phys. Rev. B* **89** (2014) 205204(1-8).
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## Wadati group

Our main experimental techniques are synchrotron-based x-ray spectroscopy and scattering. We studied the orbital and magnetic phase transitions in  $\text{Pr}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$  epitaxial thin films by resonant soft x-ray scattering and observed three phase transitions, one of which is absent in bulk  $\text{Pr}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ . We also studied the valence of Bi in Bi-based new-type superconductors by x-ray absorption spectroscopy and obtained evidence for the scenario of electron doping for the emergence of superconductivity.

1. Antiferromagnetic Order of the  $\text{Co}^{2+}$  High-Spin State with a Large Orbital Angular Momentum in  $\text{La}_{1.5}\text{Ca}_{0.5}\text{CoO}_4$ : J. Okamoto, H. Nakao, Y. Yamasaki, H. Wadati, A. Tanaka, M. Kubota, K. Horigane, Y. Murakami and K. Yamada, *J. Phys. Soc. Jpn.* **83** (2014) 044705.
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\* Joint research among groups within ISSP.

## Kondo group

We use angle-resolved photoemission spectroscopy (ARPES) with ultrahigh energy resolution, achieved by using laser photon source, and study the nonconventional superconductors, heavy fermions, strongly correlated systems, topological quantum phases, and quantum well states. The main findings in 2013 are as follows: (1) Formation of Gapless Fermi Arcs and Fingerprints of Order in the Pseudogap State of Cuprate Superconductors. (2) Anomalous Dressing of Dirac Fermions in the Topological Surface State. (3) Significant doping Variation of the Nodal Low-Energy Feature of Superconducting  $\text{Bi}_2\text{Sr}_2\text{CuO}_{6+\delta}$  ( $\text{Bi}2201$ ) crystals.

1. <sup>†\*</sup> Anomalous Doping Variation of the Nodal Low-Energy Feature of Superconducting  $(\text{Bi,Pb})_2(\text{Sr,La})_2\text{CuO}_{6+\delta}$  Crystals Revealed by Laser-Based Angle-Resolved Photoemission Spectroscopy: T. Kondo, Y. Nakashima, W. Malaeb, Y. Ishida, Y. Hamaya, T. Takeuchi and S. Shin, *Phys. Rev. Lett.* **110** (2013) 217006(1-5).
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3. Formation of Gapless Fermi Arcs and Fingerprints of Order in the Pseudogap State of Cuprate Superconductors.: T. Kondo, A. D. Palczewski, Y. Hamaya, T. Takeuchi, J. S. Wen, Z. J. Xu, G. Gu and A. Kaminski, *Phys. Rev. Lett.* **111** (2013) 157003(1-5).
4. <sup>†\*</sup> Surface electronic structure of the topological Kondo-insulator candidate correlated electron system  $\text{SmB}_6$ : M. Neupane, N. Alidoust, S. -Y. Xu, T. Kondo, Y. Ishida, D. J. Kim, C. Liu, I. Belopolski, Y. J. Jo, T. -R. Chang, H. -T. Jeng, T. Durakiewicz, L. Balicas, H. Lin, A. Bansil, S. Shin, Z. Fisk and M. Z. Hasan, *Nat. Commun.* **4** (2013) 2991(1-7).
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<sup>†</sup> Joint research with outside partners.