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 2017 include: (1) Determination of complete phase diagram of ferro qudrupole order in $PrTi_2Al_{20}$ showing remarkable anisotropy with respect to the magnetic fied direction, (2) successful explanation of the above results by mean field calculation of a model hamiltonian including field dependent anisotropic quadupole interactioin, and (3) synthesis of single crystal of the breathing pyrochlore material LiGa Cr_4O_8 followed by magnetiation and NMR measuremengs on the magnetic ordering and spin structure.

1. *Collinear spin density wave order and anisotropic spin fluctuations in the frustrated J_1-J_2 chain magnet $NaCuMoO_4(OH)$: K. Nawa, M. Yoshida, M. Takigawa, Y. Okamoto and Z. Hiroi, Phys. Rev. B **96** (2017) 174433(1-9).

2. Dynamics of bound magnon pairs in the quasi-one-dimensional frustrated magnet $LiCuVO_4$: K. Nawa, M. Takigawa, S. Krämer, M. Horvatic, C. Berthier, M. Yoshida and K. Yoshimura, Phys. Rev. B **96** (2017) 134423(1-6).

3. *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(1-9).

4. *Spin dynamics in the high-field phases of volborthite: M. Yoshida, K. Nawa, H. Ishikawa, M. Takigawa, M. Jeong, S. Krämer, M. Horvatic, C. Berthier, K. Matsui, T. Goto, S. Kimura, T. Sasaki, J. Yamaura, H. Yoshida, Y. Okamoto and Z. Hiroi, Phys. Rev. B **96** (2017) 180413(R)(1-5).

5. *Classical Spin Nematic Transition in $LiGa_{0.95}In_{0.05}Cr_4O_8$: R. Wawrzynczak, Y. Tanaka, M. Yoshida, Y. Okamoto, P. Manuel, N. Casati, Z. Hiroi, M. Takigawa and G. J. Nilsen, Phys. Rev. Lett. **119** (2017) 087201(1-6).

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 2017. (1) Field-induced ferromagnetic quantum phase transition of itinerant Ising ferromagnet URhGe has been studied by means of angle-resolved magnetization measurements. Details of the wing structure phase diagram is obtained. A tricritical point is likely to exists at ~4 K. (2) Quantum criticality of the spin-1/2 ferromagnetic-leg ladder 3-I-V [=3-(3-iodophenyl)-1,5-diphenylverdazyl] has been examined with respect to the antiferromagnetic to paramagnetic phase transition. The critical exponents of the phase boundary agreed with a theoretical prediction of the quasi-1D Bose-Einstein condensation. (3) We studied the superconducting (SC) gap symmetry and magnetic response of cubic $U_{0.97}Th_{0.03}Be_{13}$ by means of heat capacity and magnetization measurements. We confirmed that the previously-reported second phase transition is between two different SC states. Field and orientation dependences of the heat capacity indicate that the gap is fully opened over the Fermi surface.

1. †Magnetic Properties and Magnetic Phase Diagrams of Trigonal $DyNi_3Ga_9$: H. Ninomiya, Y. Matsumoto, S. Nakamura, Y. Kono, S. Kittaka, T. Sakakibara, K. Inoue and S. Ohara, J. Phys. Soc. Jpn. **86** (2017) 124704(1-7).

2. Structural, Magnetic, and Superconducting Properties of Caged Compounds ROs$_2$Zn$_{20}$ (R= La, Ce, Pr, 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).

3. *Thermodynamic Investigation of Metamagnetic Transitions and Partial Disorder in the Quasi-Kagome Kondo Lattice 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).

* Joint research among groups within ISSP.

4. Gap structure of FeSe determined by angle-resolved specific heat measurements in applied rotating magnetic field: Y. Sun, S. Kittaka, S. Nakamura, T. Sakakibara, K. Irie, T. Nomoto, K. Machida, J. Chen and T. Tamegai, Phys. Rev. B **96** (2017) 220505(1-5).

5. †Magnetic properties of the *S*=1/2 honeycomb lattice antiferromagnet 2-Cl-3,6-F_2-V: T. Okabe, H. Yamaguchi, S. Kittaka, T. Sakakibara, T. Ono and Y. Hosokoshi, Phys. Rev. B **95** (2017) 075120(1-6).

6. †Quasiparticle excitations and evidence for superconducting double transitions in monocrystalline $U_{0.97}Th_{0.03}Be_{13}$: Y. Shimizu, S. Kittaka, S. Nakamura, T. Sakakibara, D. Aoki, Y. Homma, A. Nakamura and K. Machida, Phys. Rev. B **96** (2017) 100505(1-5).

7. Three-dimensional Bose-Einstein condensation in the spin-1/2 ferromagnetic-leg ladder 3-Br-4-F-V: Y. Kono, H. Yamaguchi, Y. Hosokoshi and T. Sakakibara, Phys. Rev. B **96** (2017) 104439(1-6).

8. Wing structure in the phase diagram of the Ising ferromagnet URhGe close to its tricritical point investigated by angle-resolved magnetization measurements: S. Nakamura, T. Sakakibara, Y. Shimizu, S. Kittaka, Y. Kono, Y. Haga, J. Pospíšil and E. Yamamoto, Phys. Rev. B **96** (2017) 094411(1-9).

9. Nodal gap structure of the heavy-fermion superconductor URu_2Si_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).

10. 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).

11. †Randomness-induced quantum spin liquid on honeycomb lattice: H. Yamaguchi, M. Okada, Y. Kono, S. Kittaka, T. Sakakibara, T. Okabe, Y. Iwasaki and Y. Hosokoshi, Sci. Rep. **7** (2017) 16144(1-6).

12. *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.

13. Fully gapped superconductivity with no sign change in the prototypical heavy-fermion $CeCu_2Si_2$: T. Yamashita, T. Takenaka, Y. Tokiwa, J. A. Wilcox, Y. Mizukami, D. Terazawa, Y. Kasahara, S. Kittaka, T. Sakakibara, M. Konczykowski, S. Seiro, H. S. Jeevan, C. Geibel, C. Putzke, T. Onishi, H. Ikeda, A. Carrington, T. Shibauchi and Y. Matsuda, Sci. Adv. **3** (2017) e1601667(1-7).

14. Giant Hall Resistivity and Magnetoresistance in Cubic Chiral Antiferromagnet EuPtSi: M. Kakihana, D. Aoki, A. Nakamura, F. Honda, M. Nakashima, Y. Amako, S. Nakamura, T. Sakakibara, M. Hedo, T. Nakama and Y. Onuki, J. Phys. Soc. Jpn. **87** (2018) 023701(1-4).

15. Magnetic-field-induced Quantum Phase in S = 1/2 Frustrated Trellis Lattice: H. Yamaguchi, D. Yoshizawa, T. Kida, M. Hagiwara, A. Matsuo, Y. Kono, T. Sakakibara, Y. Tamekuni, H. Miyagai and Y. Hosokoshi, J. Phys. Soc. Jpn. **87** (2018) 043701(1-5).

16. Quasi-one-dimensional Bose-Einstein condensation in the spin-1/2 ferromagnetic-leg ladder 3-I-V: Y. Kono, S. Kittaka, H. Yamaguchi, Y. Hosokoshi and T. Sakakibara, Phys. Rev. B **97** (2018) 100406(1-5).

17. Fermi surface in the absence of a Fermi liquid in the Kondo insulator SmB_6: M. Hartstein, W. H. Toews, Y. -T. Hsu, B. Zeng, X. Chen, M. Ciomaga Hatnean, Q. R. Zhang, S. Nakamura, A. S. Padgett, G. Rodway-Gant, J. Berk, M. K. Kingston, G. H. Zhang, M. K. Chan, S. Yamashita, T. Sakakibara, Y. Takano, J. -H. Park, L. Balicas, N. Harrison, N. Shitsevalova, G. Balakrishnan, G. G. Lonzarich, R. W. Hill, M. Sutherland and S. E. Sebastian, Nature Phys. **14** (2018) 166-172.

18. †*Quantum valence criticality in a correlated metal: K. Kuga, Y. Matsumoto, M. Okawa, S. Suzuki, T. Tomita, K. Sone, Y. Shimura, T. Sakakibara, D. Nishio-Hamane, Y. Karaki, Y. Takata, M. Matsunami, R. Eguchi, M. Taguchi, A. Chainani, S. Shin, K. Tamasaku, Y. Nishino, M. Yabashi, T. Ishikawa and S. Nakatsuji, Sci. Adv. **4** (2018) eaao3547 (1-6).

19. 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.

Mori group

We have successfully developed and unveiled unprecedented functional properties for the molecular materials. The major achievements in 2017 are (1) to disclose the "proton-electron coupled properties" such as quantum spin liquid and H/D isotope

† Joint research with outside partners.

effects for our developed organic conductor, κ-H_3(Cat-EDT-TTF)$_2$, by the measurements of specific heat, dielectric response, and thermal conductivity, and DFT calculation, (2) to develop and reveal the peculiarities for novel hydrogen-bonded organic conductors, β-[BTBT(OH)$_2$]$_2$$ClO_4$ and β'-H_3(Cat-EDO-TTF)$_2$$BF_4$, and (3) to demonstrate the "charge-glass" in organic conductor, θ-(BEDT-TTF)$_2$TlZn(SCN)$_4$.

1. Thermodynamics of the quantum spin liquid state of the single-component dimer Mott system κ–H_3(Cat–EDT–TTF)$_2$: S. Yamashita, Y. Nakazawa, A. Ueda and H. Mori, Phys. Rev. B **95** (2017) 184425(1-5).

2. Visualization of a nonlinear conducting path in an organic molecular ferroelectric by using emission of terahertz radiation: M. Sotome, N. Kida, Y. Kinoshita, H. Yamakawa, T. Miyamoto, H. Mori and H. Okamoto, Phys. Rev. B **95** (2017) 241102R(1-5).

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) 3426-3429.

4. Crystallization and vitrification of electrons in a glass-forming charge liquid: S. Sasaki, K. Hashimoto, R. Kobayashi, K. Itoh, S. Iguchi, Y. Nishio, Y. Ikemoto, T. Moriwaki, N. Yoneyama, M. Watanabe, A. Ueda, H. Mori, K. Kobayashi, R. Kumai, Y. Murakami, J. Müller and T. Sasaki, Science **357** (2017) 1381-1385.

5. Multicomponent DFT study of geometrical H/D isotope effect on hydrogen-bonded organic conductor, κ-H_3(Cat EDT-ST)$_2$: K. Yamamoto, Y. Kanematsu, U. Nagashima, A. Ueda, H. Mori and M. Tachikawa, Chem. Phys. Lett. **674** (2017) 168-172.

6. [*]Quantum-disordered state of magnetic and electric dipoles in an organic Mott system: M. Shimozawa, K. Hashimoto, A. Ueda, Y. Suzuki, K. Sugii, S. Yamada, Y. Imai, R. Kobayashi, K. Itoh, S. Iguchi, M. Naka, S. Ishihara, H. Mori, T. Sasaki and M. Yamashita, Nat. Commun. **8** (2017) 1821(1-6).

7. 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) 367-375.

8. 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) 1449-1453.

9. Spin-Singlet Transition in the Magnetic Hybrid Compound from a Spin-Crossover Fe(III) Cation and π-Radical Anion: K. Takahashi, T. Sakurai, W.-M. Zhang, S. Okubo, H. Ohta, T. Yamamoto, Y. Einaga and H. Mori, Inorganics **5** (2017) 54(1-14).

10. Development of Novel Functional Organic Crystals by Utilizing Proton- and π-Electron-Donating/Accepting Abilities: A. Ueda, Bull. Chem. Soc. Jpn **90** (2017) 1181-1188.

11. Antiferromagnetic Ordering in Organic Conductor λ-(BEDT-TTF)$_2$$GaCl_4$ Probed by ^{13}C NMR: Y. Saito, S. Fukuoka, T. Kobayashi, A. Kawamoto and H. Mori, J. Phys. Soc. Jpn. **87** (2018) 013707(1-4).

12. Size effects on supercooling phenomena in strongly correlated electron systems: $IrTe_2$ and θ-(BEDT-TTF)$_2$RbZn(SCN)$_4$: H. Oike, M. Suda, M. Kamitani, A. Ueda, H. Mori, Y. Tokura, H. M. Yamamoto and F. Kagawa, Phys. Rev. B **97** (2018) 085102(1-7).

13. [†*]Strong Hydrogen Bonds at the Interface between Proton-Donating and -Accepting Self-Assembled Monolayers on Au(111): H. S. Kato, S. Yoshimoto, A. Ueda, S. Yamamoto, Y. Kanematsu, M. Tachikawa, H. Mori, J. Yoshinobu and I. Matsuda, Langmuir **34** (2018) 2189-2197.

14. The thermoelectric power of band-filling controlled organic conductors, β′-(BEDT-TTF)$_3$$(CoCl_4)_{2-x}$$(GaCl_4)_x$: Y. Kiyota, T. Kawamoto, H. Mori and T. Mori, J. Mater. Chem. A **6** (2018) 2004-2010.

15. A phenol-fused tetrathiafulvalene: modulation of hydrogen-bond patterns and electrical conductivity in the charge-transfer salt: A. Ueda and H. Mori, Mater. Chem. Front. **2** (2018) 566-572.

16. Anisotropic Proton Conductivity Arising from Hydrogen-Bond Patterns in Anhydrous Organic Single Crystals, Imidazolium Carboxylates: Y. Sunairi, A. Ueda, J. Yoshida, K. Suzuki and H. Mori, J. Phys. Chem. C (2018), in print.

Osada group

A layered organic Dirac semimetal α-(BEDT-TTF)$_2$$I_3$ shows a metal-insulator transition due to charge ordering (CO) at ambient pressure, which is suppressed by applying pressure. We found that its temperature dependence of resistance below the CO transition shows no insulating behavior but metallic behavior in the weak CO state just below the critical pressure (~ 1.1 GPa).

[*] Joint research among groups within ISSP.

We investigated the temperature dependence of magnetoresistance in detail, and concluded that the gapped Dirac fermion state is realized in the weak CO state. Based on these experimental result, we consider the electronic structure of α-(BEDT-TTF)$_2$I$_3$ with intracellular potential and magnetic modulations due to CO, which were observed in NMR measurement. This is an organic analogue of the Haldane model in graphene. When magnetic modulation is sufficiently large, the system becomes a Chern insulator, where the Berry curvatures around two gapped Dirac cones have the same sign on each band, and one chiral edge state connects the conduction and valence bands at each crystal edge. We pointed out the possibility that the metallic transport in the weak CO state originates from the edge transport in the Chern insulator state.

1. Chern Insulator Phase in a Lattice of an Organic Dirac Semimetal with Intracellular Potential and Magnetic Modulations: T. Osada, J. Phys. Soc. Jpn. **86** (2017) 123702(1-5).

2. Topological Insulator State due to Finite Spin-Orbit Interaction in an Organic Dirac Fermion System: T. Osada, J. Phys. Soc. Jpn. **87** (2018) 075002(1-2).

3. Thickness-dependent phase transition in graphite under high magnetic field: T. Taen, K. Uchida and T. Osada, Phys. Rev. B **97** (2018) 115122(1-7).

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 $CeCoIn_5$ at ultra-low temperatures, (2) thermal Hall measurements of kagome materials and (3) scanning-Hall measurements of Mn_3Sn and Fe-based superconductors.

1. *Thermal Hall Effect in a Phonon-Glass $Ba_3CuSb_2O_9$: 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(1-5).

2. *Quantum-disordered state of magnetic and electric dipoles in an organic Mott system: M. Shimozawa, K. Hashimoto, A. Ueda, Y. Suzuki, K. Sugii, S. Yamada, Y. Imai, R. Kobayashi, K. Itoh, S. Iguchi, M. Naka, S. Ishihara, H. Mori, T. Sasaki and M. Yamashita, Nat. Commun. **8** (2017) 1821(1-6).

3. Anomalous Change in the de Haas–van Alphen Oscillations of $CeCoIn_5$ at Ultralow Temperatures: H. Shishido, S. Yamada, K. Sugii, M. Shimozawa, Y. Yanase and M. Yamashita, Phys. Rev. Lett. **120** (2018) 177201.

4. 格子振動による熱ホール効果：杉井か おり , 山下 穣 , 固体物理 **52** (2017) 783.

Division of Condensed Matter Theory

Tsunetsugu group

We have investigated the antiferromagnetic order in a quasicrystal from the viewpoint of the interplay between strong correlation effects and unique crystal structure. To this end, we have employed the simplest canonical model, i.e. the Hubbard model on the two-dimensional Penrose lattice at half filling of electron density. Due to the quasiperiodic lattice structure, this model has thermodynamically degenerate one-electron states at the band center. Each of their wavefunctions is confined in a finite region in the lattice, and thereofre they are called the confined states. These confined states are magnetized by Coulomb repulsion between electrons. They show an antiferromagnetic long-range order at zero temperature, but its spatial structure differs from other antiferromagnets. The whole Penrose lattice is divided into many clusters, and the ordered magnetizations point to the same direction in each cluster, while neighboring clusters have opposite directions each other. Furthermore, the cluster size exhibits a power-law distribution, which is related to the self-similarity in the lattice inherent from the quasiperiodicity.

1. Antiferromagnetic order in the Hubbard model on the Penrose lattice: A. Koga and H. Tsunetsugu, Phys. Rev. B **96** (2017) 214402.

2. 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).

3. Theory of antiferromagnetic Heisenberg spins on a breathing pyrochlore lattice: H. Tsunetsugu, Prog. Theor. Exp. Phys. **2017** (2017) 033101(1-29).

4. Entanglement prethermalization in the Tomonaga-Luttinger model: E. Kaminishi, T. Mori, T. N. Ikeda and M. Ueda, Phys. Rev. A **97** (2018) 013622(1-9).

† Joint research with outside partners.

Kato group

The main research subject of Kato lab. is theory of non-equilibrium properties in mesoscopic devices. We have studied (1) spin-current noise at the interface between a ferromagnetic insulator and a metal, (2) effect of Coulomb interaction on charge pumping via a quantum dot due to reservoir temperature driving, (3) heat transport via a two-state system, and (4) current correlations of a Kondo correlated dot with degenerated orbitals. In collaboration with Sugino group, we have studied first-principles description of van der Waals bonded spin-polarized systems such as solid oxygen using the vdW-DF+U method. We have also studied terahertz response of a ferromagnetic insulator $ErFeO_3$ in collaboration with an experimental group (Suemoto group).

1. Temperature-Driven and Electrochemical-Potential-Driven Adiabatic Pumping via a Quantum Dot: M. Hasegawa and T. Kato, J. Phys. Soc. Jpn. **86** (2017) 024710(1-13).
2. [*]First-principles description of van der Waals bonded spin-polarized systems using the vdW-DF+U method: Application to solid oxygen at low pressure: S. Kasamatsu, T. Kato and O. Sugino, Phys. Rev. B **95** (2017) 235120(1-11).
3. 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(1-5).
4. Observation of long-lived coherent spin precession in orthoferrite $ErFeO_3$ induced by terahertz magnetic fields: H. Watanabe, T. Kurihara, T. Kato, K. Yamaguchi and T. Suemoto, Appl. Phys. Lett. **111** (2017) 092401(1-4).
5. 多端子系のジョセフソン接合が示すトポロジカル物性：横山 知大 , 日本物理学会誌 **72** (2017) 402.
6. Effect of Interaction on Reservoir-Parameter-Driven Adiabatic Charge Pumping via a Single-Level Quantum Dot System: M. Hasegawa and T. Kato, J. Phys. Soc. Jpn. **87** (2018) 044709.
7. Current cross-correlation in the Anderson impurity model with exchange interaction: R. Sakano, A. Oguri, Y. Nishikawa and E. Abe, Phys. Rev. B **97** (2018) 045127(1-13).
8. Spin Current Noise of the Spin Seebeck Effect and Spin Pumping: M. Matsuo, Y. Ohnuma, T. Kato and S. Maekawa, Phys. Rev. Lett. **120** (2018) 235120(1-5).
9. 物質科学シミュレーションのポータルサイト MateriApps: 本山 裕一 , 三澤 貴宏 , 加藤 岳生 , 藤堂 眞治 , 固体物理 **52** (2017) 743.
10. 非平衡電流ゆらぎでみる量子ドットの電子多体効果：阪野 塁 , 物性研究・電子版 **6** (2017) 064208.

Division of Nanoscale Science

Katsumoto group

Physical properties of quantum Hall edge states have been unveiled through thermoelectric power caused by microwave irradiation. Study on the effect of decoration on the surfaces of graphene or other 2D materials has been going on. We found strong ferromagnetism in MoS_2 with nano-mesh. Also large spin orbit interaction was introduced with nano-particles on graphene. A peculiar phenomenon called Zitterbewegung theoretically found long time ago by Schrodinger was observed as reproducible conductance fluctuation in spin-polarized transport through a two-dimensional electrons with strong Rashba-type spin-orbit interaction.

1. [†]Theoretical modeling of electrical resistivity and Seebeck coefficient of bismuth nanowires by considering carrier mean free path limitation: M. Murata, A. Yamamoto, Y. Hasegawa, T. Komine and A. Endo, J. Appl. Phys. **121** (2017) 014303 (1-10).
2. [†]Photoresponse in gate-tunable atomically thin lateral MoS_2 Schottky junction patterned by electron beam: Y. Katagiri, T. Nakamura, C. Ohata, S. Katsumoto and J. Haruyama, Appl. Phys. Lett. **110** (2017) 143109(1-3).
3. 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) 1755-1767.
4. Observation of Conductance Fluctuation due to Zitterbewegung in InAs 2-dimentional Electron Gas: Y. Iwasaki, Y. Hashimoto, T. Nakamura and S. Katsumoto, J. Phys.: Conf. Ser. **864** (2017) 012054(1-4).
5. Edge-spin-derived magnetism in few-layer MoS_2 nanomeshes: G. Kondo, N. Yokoyama, S. Yamada, Y. Hashimoto, C. Ohata, S. Katsumoto and J. Haruyama, AIP Advances **7** (2017) 125019(1-7).

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[*] Joint research among groups within ISSP.

6. Conductance fluctuations in InAs quantum wells possibly driven by Zitterbewegung: Y. Iwasaki, Y. Hashimoto, T. Nakamura and S. Katsumoto, Sci. Rep. **7** (2017) 7909(1-9).

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.

8. Frequencies of the Edge-Magnetoplasmon Excitations in Gated Quantum Hall Edges: A. Endo, K. Koike, S. Katsumoto and Y. Iye, J. Phys. Soc. Jpn. **87** (2018) 064709.

9. Frequency dependent ac transport of films of close-packed carbon nanotube arrays: A. Endo, S. Katsumoto, K. Matsuda, W. Norimatsu and M. Kusunoki, J. Phys.: Conf. Ser. **969** (2018) 012129.

10. Proximity-Induced Superconductivity in a Ferromagnetic Semiconductor (In,Fe)As: T. Nakamura, L. D. Anh, Y. Hashimoto, Y. Iwasaki, S. Ohya, M. Tanaka and S. Katsumoto, J. Phys.: Conf. Ser. **969** (2018) 012036.

Otani group

We have studied following topics this year: Spin conversion behaviors at the interfaces and the surfaces, magnetization dynamics in ferromagnetic nano structures, and magneto-thermoelectric properties. In the first topic, we succeeded in optically detect spin accumulation induced at the copper/Bi oxide interface. We have performed collaborative study with Tokura-group at CEMS RIKEN on non-linear Hall effect and spin orbit torque induced magnetization switching in magnetic topological insulator. Spin transport in a ferromagnet is also an important topic in relation with spin conversion, we have applied our spin absorption technique to determine the spin diffusion length of Ni-Fe alloy nano wires. In the second topic, we have established the technique to modulate the interface perpendicular anisotropy by voltage. Thereby we succeeded in exciting coherent propagating spin waves in ultrathin CoFeB films. In the third topic, we have found bulk equivalent anomalous Nernst effect takes place in a microfabricated thermoelectric element made of chiral antiferromagnet Mn_3Sn in collaboration with Nakatsuji group.

1. Bias field tunable magnetic configuration and magnetization dynamics in $Ni_{80}Fe_{20}$ nano-cross structures with varying arm length: K. Adhikari, S. Choudhury, R. Mandal, S. Barman, Y. Otani and A. Barman, J. Appl. Phys. **121** (2017) 043909(1-5).

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4. *Anomalous Nernst effect in a microfabricated thermoelectric element made of chiral antiferromagnet Mn_3Sn: H. Narita, M. Ikhlas, M. Kimata, A. A. Nugroho, S. Nakatsuji1 and Y. Otani, Appl. Phys. Lett. **111** (2017) 202404(1-5).

5. Direct optical observation of spin accumulation at nonmagnetic metal/oxide interface: J. Puebla, F. Auvray, M. Xu, B. Rana, A. Albouy, H. Tsai, K. Kondou, G. Tatara and Y. Otani, Appl. Phys. Lett. **111** (2017) 092402(1-4).

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Komori group

A-few-atomic-layer ferromagnetic γ'-Fe4N thin films are studied by scanning tunneling microscopy/spectroscopy (STM/STS) and soft X-ray magnetic circular dichroism. The spin magnetic moment of Fe atoms increases with increasing the average thickness reaching 1.4μ_B/atom in the trilayer sample. Hexagonal atomic- layer iron nitrides with different crystal and local electronic structures are also found to grow on the Cu(001) surface. Local change of the electron-phonon coupling in periodically nano-modulated graphene on a macrofacet of SiC(0001) substrate is studied using inelastic STS. The coupling depends on the local distance between the graphene and the SiC substrate. An in-gap surface state on a Kondo insulator SmB_6(001) surface is studied by STS. The surface state survives even on the area with significant density of defects, which supports the existence of the topological Kondo surface state on this surface.

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19. †Evaluation of structural vacancies for 1/1-Al–Re–Si approximant crystals by positron annihilation spectroscopy: K. Yamada, H. Suzuki, H. Kitahata, Y. Matsushita, K. Nozawa, F. Komori, R. S. Yu, Y. Kobayashi, T. Ohdaira, N. Oshima, R. Suzuki, Y. Takagiwa, K. Kimura and I. Kanazawa, Philos. Mag. **98** (2018) 107-117.

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Hasegawa group

Using low-temperature ultrahigh vacuum scanning tunneling microscopy (STM) we have obtained real-space images showing orbital order on a Co-terminated surface of $CeCoIn_5$, which is a heavy-fermion superconducting material. Because of the 4-fold symmetry regardless of the sites in the bulk or on the surface, $3d_{xz}$ and $3d_{yz}$ orbitals of the Co atoms are energetically degenerated. However, on the surface, because of the reduced coordination number and resulting enhanced electron correlation, the capability of the electron screening is suppressed. As a result, in order to reduce the Coulomb repulsive energy alternating unoccupation among the two 3*d* orbitals in an antiferromagnetic manner becomes favorable on the surface. We observed alternately-arranged dumbbell shapes whose shape is quite similar with that of d_{xz} and d_{yz} orbitals looking from the z direction, proving the existence of the orbital order. In a technical point of view of STM, observing d orbitals is not an easy task because of their localized nature near the core. Since STM detects wave functions of sample surface by the probe tip, states that

† Joint research with outside partners.

decay long from the surface are probed more efficiently than quickly decaying states. In fact, on the Co-terminated surface we observed round-shaped Co atoms arranged in a square lattice in standard tunneling conditions, which obviously originate from *s*-derived states of Co. In order to observe the d orbitals, we intentionally locate the tip near the surface almost touching to the surface but still in the tunneling regime, and successfully observed their ordering, which had not been achieved before. In 2017, we also performed collaborative research works with in-house, domestic, and oversea groups, some of which were published in high-impact journals. We have obtained STM images of a monolayer boron film called borophene in collaboration with Prof. Iwao Matsuda, ISSP, and Fe phthalocyanine molecules adsorbed on silicene in collaboration with Prof. Yamada-Takamura, JAIST and Prof. Hirjibehedin, University College London. We also performed study on atomically controlled point contact formation with Prof. Sakai, Kyoto University.

1. †Break voltage of Au single-atom contacts formed by junction closure: S. Wakasugi, S. Kurokawa, H. Kim, Y. Hasegawa and A. Sakai, J. Appl. Phys. **121** (2017) 244304(1-8).

2. 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).

3. †*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).

4. †Guided Molecular Assembly on a Locally Reactive 2D Material: B. Warner, T. G. Gill, V. Caciuc, N. Atodiresei, A. Fleurence, Y. Yoshida, Y. Hasegawa, S. Blügel, Y. Yamada-Takamura and C. F. Hirjibehedin, Adv. Mater. **29** (2017) 1703929(1-7).

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6. Atomic-scale visualization of surface-assisted orbital order: H. Kim, Y. Yoshida, C.-C. Lee, T.-R. Chang, H.-T. Jeng, H. Lin, Y. Haga, Z. Fisk and Y. Hasegawa, Sci. Adv. **3** (2017) eaao0362(1-5).

Lippmaa group

The main research topics for this year concerned energy conversion materials used for photoelectrochemical water splitting. We studied the initial growth phase of Ir:$SrTiO_3$ and found that nanoscale Ir-rich clusters nucleate at the beginning of film growth, ultimately leading to macroscopic segregation of metal nanopillars. We also studied the growth characteristics of IrO_2 films, mapping the stability phase diagram for Ir oxides and worked on fabricating a potential topological pyrochlore iridate phase, $Pr_2Ir_2O_7$.

1. 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ー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ー： 高橋竜太 , リップ マーミック , 固体物理 **52** (2017) 105-116.

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3. Microstructure analysis of IrO_2 thin films: X. Hou, R. Takahashi, T. Yamamoto and M. Lippmaa, J. Cryst. Growth **462** (2017) 24-28.

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8. 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).

9. Thermally Stable Sr_2RuO_4 Electrode for Oxide Heterostructures: R. Takahashi and M. Lippmaa, ACS Appl. Mater. Interfaces **9** (2017) 21314–21321.

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* Joint research among groups within ISSP.

10. Pyroelectric detection of ferroelectric polarization in magnetic thin films: R. Takahashi and M. Lippmaa, Jpn. J. Appl. Phys. **57** (2018) 0902A1.

11. †Noble metal nanocluster formation in epitaxial perovskite thin films: M. Lee, R. Arras, R. Takahashi, B. Warot-Fonrose, H. Daimon, M.-J. Casanove and M. Lippmaa, ACS Omega **3** (2018) 2169-2173.

12. 酸化物半導体中に自己組織化した金属ナノピラーによる高効率・水分解光電極反応 : 川崎 聖治 , 高橋 竜太 , リップマー ミック , 応用物理 **87** (2018) 366-369.

Functional Materials Group

Yoshinobu group

We conducted several research projects in the fiscal year 2017: (1) Systematic study of the activation and hydrogenation of CO_2 on Cu model catalysts by AP-XPS, IRAS, and TPD. (2) The surface chemistry of formic acid on Cu model catalysts studied by SR-PES, IRAS and TPD. (3) Spectroscopic characterization of Pd-Cu and Pd-Ag surfaces by XPS. (4) Spectroscopic characterization of adsorption and thermal processes of NO on silicone/ZrB_2/Si(111) using SR-XPS. (5) LT-STM study of Zn on Cu(997). (6) Independently driven four-probe conductivity measurement of organic thin films and organic single crystals.

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4. †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, Surf. Sci. **663** (2017) 1–10.

5. *Adsorption of CO_2 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) 2807-2814.

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7. †*Strong Hydrogen Bonds at the Interface between Proton-Donating and -Accepting Self-Assembled Monolayers on Au(111): H. S. Kato, S. Yoshimoto, A. Ueda, S. Yamamoto, Y. Kanematsu, M. Tachikawa, H. Mori, J. Yoshinobu and I. Matsuda, Langmuir **34** (2018) 2189-2197.

8. Initial gas exposure effects on monolayer pentacene field-effect transistor studied using four gallium indium probes: S. Yoshimoto, R. Miyahara, Y. Yoshikura, J. Tang, K. Mukai and J. Yoshinobu, Org. Electron. **54** (2018) 34-39.

Akiyama group

In 2017, we started fabrication of 1035nm InGaAs laser diodes for short and intense pulse generation via gain switching. In parallel, we studied pico- and femto-second short-pulse generation and pulse dynamics in GaAs, GaN, and other semiconductor gain-switched lasers via optical pumping and current injection. We studied single- and multi-junction solar cells by absolute electroluminescence-efficiency measurement methods, and via time-resolved photo-emission spectroscopy, we studied photo-voltage dynamics solar cells after impulsive optical excitations. We made computational studies with quantum-chemistry and molecular-dynamics calculations on oxyluciferins and caged-luciferins.

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† Joint research with outside partners.

2. 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(1-5).

3. "Visible" 5d orbital states in a pleochroic oxychloride: D. Hirai, T. Yajima, D. Nishio-Hamane, C. Kim, H. Akiyama, M. Kawamura, T. Misawa, N. Abe, T.-H. Arima and Z. Hiroi, J. Am. Chem. Soc. **139** (2017) 10784-10789.

4. Picosecond tunable gain-switched blue pulses from GaN laser diodes with nanosecond current injections: S. Chen, T. Nakamura, T. Ito, H. Nakamae, X. Bao, G. Weng, X. Hu, M. Yoshita, H. Akiyama, J. Liu, M. Ikeda and H. Yang, Opt. Express **25** (2017) 13046-13054.

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Sugino group

We have made progress in functional matter research of (1) electrocatalysis, (2) oxygen solid, (3) hidroxyapatite, (4) bio-luminescence, and (5) monolayer Dirac materials. We have also developed methods for (a) many-body Green's function calculation and (b) tensor decomposition of many-body wave function.

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Quantum Materials Group

Oshikawa group

We studied a wide range of theoretical problems in condensed matter physics and statistical physics. As a novel application of anomaly in quantum field theory, we discussed possible gapless critical phases of quantum antiferromagnetic chains with general spin quantum numbers. The critical theory with the exact SU(2) symmetry and the emergent Lorentz invariance has been classified by the SU(2) Wess-Zumino-Witten (WZW) theories labeled by a natural number called level. We found that, in the presence of the translation symmetry, even- and odd-level WZW theories can be only realized in integer- and half-odd-integer spin chains, respectively. This follows from an anomaly matching and can be regarded as a field-theory manifestation of the Lieb-Schultz-Mattis constraint. The present result leads to a novel concept of "symmetry-protected critical phases".

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Nakatsuji group

Our group explores ground state properties and spintronic functions of novel quantum phases and phase transitions in rare-earth and transition metal based compounds. The followings are some relevant results obtained in 2017. (1) We discovered the anomalous Nernst effect for the first time in an antiferromagnet. Strikingly, the effect in the antiferromagnet Mn_3Sn is found more than 100 times larger than the estimate based on its magnetization. (2) We discovered the first example of a Weyl magnet. In particular, we found strong experimental evidence for the Weyl fermions in the antiferromagnet Mn_3Sn. (3) We discovered the magneto optical Kerr effect for the first time in an antiferromagnetic metal. We observed a large zero-field Kerr rotation angle ~ 20 mdeg and a clear square hysteresis loop in Mn_3Sn at room temperature by the magneto-optical Kerr effect, indicating the ferroic ordering of magnetic octupoles. (4) We discovered the first example of a quantum valence transition and its quantum criticality in a metal, in particular, in the mixed valent system a-$YbAl_{1-x}Fe_xB_4$. (5) We observed a very large dielectric constant due to the strong correlation effects in the Luttinger semimetal state of $Pr_2Ir_2O_7$ using the thin films.

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Materials Design and Characterization Laboratory

Hiroi group

A new oxychloride, $Ca_3ReO_5Cl_2$, is found, which shows unusually distinct pleochroism; that is, the material exhibits different colors depending on the viewing direction. This pleochroism is a consequence of the coincidental complex crystal field splitting of the 5*d* orbitals of the Re^{6+} ion in a square-pyramidal coordination of low symmetry in the energy range of the visible spectrum. Since the relevant d–d transitions show characteristic polarization dependence according to the optical selection rule, the orbital states are "visible" in $Ca_3ReO_5Cl_2$. The superconducting pyrochlore oxide Cd2Re2O7 is revisited with a particular emphasis on the sample-quality issue. Recently, it has attracted increasing attention as a candidate spin–orbit coupled metal (SOCM), in which specific Fermi liquid instability is expected to lead to an odd-parity order with spontaneous inversion-symmetry breaking and parity-mixing superconductivity.

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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 2017 include: (1) numerical simulation of weak-first order phase transition, (2) tensor-network calculation of the frustrated magnet on the star-lattice, (3) development of methods of computing high-order magnetic moments, and (4) tensor-network calculation of spin-orbit coupled systems.

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Uwatoko group

We report the effect of hydrostatic pressure on the electronic state of the antiferromagnet UIrGe, which is isostructural and isoelectronic with the ferromagnetic superconductors UCoGe and URhGe. We constructed a p–T phase diagram and estimated the critical pressure pc, where the antiferromagnetism vanishes, as ~12 GPa. Electrical resistivity measurements have been performed on the iron-based ladder compounds $Ba_{1-x}Cs_xFe_2Se_3$ (x = 0, 0.25, 0.65, and 1) under high pressure. Metallic behavior of the electrical conductivity was confirmed in the x = 0.25 and 0.65 samples for pressures greater than 11.3 and 14.4 GPa, respectively, with the low-temperature log T upturn being consistent with weak localization of 2D electrons due to random potential. No metallic conductivity was observed in the parent compounds $BaFe_2Se_3$ (x = 0) up to 30.0 GPa and $CsFe_2Se_3$ (x = 1) up to 17.0 GPa. We report pressure-driven superconductivity (SC) in the vicinity of a commensurate charge-density wave (CCDW) in transition-metal dichalcogenides (TMDs) 1T−TaSe2 by simultaneous resistivity and ac susceptibility. The findings reveal the interplay of CCDW and SC in 1T−$TaSe_2$ by a clean method, viz., high pressure, and shed light on the underlying superconducting mechanism in the relevant systems. We study the properties of electronic structure in the high-Tc phase induced by pressure in bulk FeSe from magnetotransport measurements and first-principles calculations. These results in FeSe highlight similarities with high-Tc phases of iron pnictides, constituting a step toward a unified understanding of iron-based superconductivity. The origin of the highly anisotropic superconducting transition in $ZrTe_3$, where the resistance along the a axis, R_a , is reduced at 4 K but those along the b axis, R_b, and c' axis, $R_{c'}$, are reduced at 2 K, was explored with the application of a magnetic field and pressure by the electrical resistance measurements. The reduction in Ra is due to filamentary supercon-

† Joint research with outside partners.

ductivity (SC) induced by locally bound electron pairs (local pairs), which correspond to bi-polarons, and the transition of R_b corresponds to the emergence of bulk SC originating from the Cooper pairs triggered by the transfer of the local pairs. We have studied the temperature-pressure phase diagram of two materials $Eu_{3-x}Sr_xBi_2S_4F_4$ (x = 1 and x = 2) by electrical resistivity and magnetic measurements down to 2 K. Using the Arrhenius equation, we estimate the thermally activated flux flow activation energy U 0 as 116 K in $Eu_2SrBi_2S_4F_4$ and 39 K in $EuSr_2Bi_2S_4F_4$. At 2 K, DC magnetic susceptibility measurements indicate S-type paramagnetic behavior. We construct the three-dimensional electronic phase diagram, temperature (T) against pressure (P) and isovalent S-substitution (x), for $FeSe_{1-x}S_x$. The completed phase diagram uncovers that high-T_c superconductivity lies near both ends of the dome-shaped antiferromagnetic phase, whereas T_c remains low near the nematic critical point.

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Ozaki group

Motivated by the post-K computer project where the machine is expected to consist of about 10 million CPU cores, we have tried to develop efficient and accurate O(N) methods whose computational cost is proportional to the number of atoms, while so far we have already developed an O(N) Krylov subspace and applied the method to a wide variety of problems. A missing ingredient in the O(N) Krylov subspace method is that the method neglects the effect of outer region beyond the truncated cluster. To take account of the effect of outer region beyond the truncated cluster, we have introduced the self-energy correction, which is derived from a block formalism for the inverse calculation of a matrix, to evaluation of local Green's function and performed a series of benchmark calculations. Though the method is theoretically appealing, it turns out that the method is numerically very unstable in the process for the self-consistent calculation of local Green's functions. The analysis implies that the Green's functions near the real axis are highly delocalized for systems with metallic bands or denser structures, resulting in the numerical instability. After getting the negative result, we have taken another direction for development of efficient and accurate O(N) methods, and considered how the size of truncated cluster can be enlarged without largely increasing the numerical cost. Our idea is based on a coarse graining of basis functions which are located in the buffer region of the truncated cluster. To perform the coarse graining, we have developed a novel method to generate localized natural orbitals based on Schur decomposition, and replaced the original basis functions in the buffer region by the localized natural orbitals. A series of benchmark calculations suggests that the O(N) method is a stable and accurate method for not only insulators but also metals. We have further introduced a multi-level parallelization where atoms, spin, and eigenvalue problem for the truncated cluster are fully parallelized by MPI. We expect that the parallelized code for the novel method enables us to perform first-principles molecular dynamics simulations of large-scale systems consisting of ten thousand atoms by making full use of the post-K computer.

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Noguchi group

We have studied the membrane shape transformations by proteins and chemical reactions. (1) Two types of banana-shaped proteins assembled into striped bumps that surpress membrane tubulation. (2) The tubulation is promoted by laterally isotropic membrane inclusions that generate the same sign of spontaneous curvature as the adsorbed protein rods while it is surpressed in the case of the opposite sign. (3) Asymmetric chemical reactions between the inner and outer leaflets of a vesicle induces bilayer sheet protrusion and budding. The probabilities of these two types of transformations depend on the shear viscosity of the surrounding fluids compared to the membrane as well as the reaction rates.

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Materials Synthesis and Characterization group

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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, 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 2017 include investigation of (1) structural investigations of critical clusters and their biomedical applications, (2) probe diffusion of sol-gel transition in isorefractive indexed solvents, (3) solvated structure of cellulose in a phosphonate-based ionic liquid, (4) structure-mechanical property relationships in crosslinked phenolic resin, and (5) structural investigations of nonswellable thermoresponsive amphiphilic conetwork, and so on.

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5. Mesoscopic Structural Aspects of Ca^{2+}-Triggered Polymer Chain Folding of a Tetraphenylethene-Appended Poly(acrylic acid) in Relation to Its Aggregation-Induced Emission Behavior: K. Morishima, F. Ishiwari, S. Matsumura, T. Fukushima and M. Shibayama, Macromolecules **50** (2017) 5940-5945.

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† Joint research with outside partners.

Yoshizawa group

A systematic study on a family of Ce-based non-centrosymmetric heavy fermion compounds $CeTSi_3$ (T=transition metal ions) was continued in 2017. It is found that a family of the $CeTSi_3$ compounds can be classified into three different crystalline electric field (CEF) level scheme groups. In order to elucidate megnetic properties from a microscopic basis, the CEF levels were reexamined for T= Rh and Ir compounds with use of inelastic neutron scattering (INS) measurements. The results disclosed that the previously reported CEF level schemes for $CeRhSi_3$ and $CeIrSi_3$ were not correct, and our INS study established the correct CEF schemes which can consistently explain other magnetic properties.

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2. †Magnetic and Thermodynamic Studies on the Charge and Spin Ordering in the highly-doped $La_{2-x}Sr_xCoO_4$: M. Yoshida, D. Ueta, Y. Ikeda, T. Yokoo, S. Itoh and H. Yoshizawa, Physica B **536** (2018) 338-341.

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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. Following to the synchrotron X-ray diffraction works of last year on the vapor-deposited glasses of carbon disulfide (CS_2), propane ($CH_3CH_2CH_3$) and propene (CH_3CHCH_2), their liquid states were measured as functions of temperature. We obtained the atomic pair distribution functions of these liquids and found that the orientational correlation between neighboring molecules steeply increases on cooling down to the glass transition temperature. This result clearly corresponds to the growth of the cooperatively rearranging region (CRR) determined by our previous calorimetric studies. Another topic is the quasielastic neutron scattering of alkylated tetraphenylporphirins (3,5-C_6C_{10}-TPP and 2,5-C_6C_{10}-TPP) whose liquid states are stabilized by the huge entropy due to the orientational disorder of alkylchains. Their molecular motions were reproduced well by the combination of the alkyl motions and the rotational and translational motions of whole molecules. Other than above topics, we have conducted neutron diffraction experiments of the nanoparticles of PdRuX (X = Pt, Rh, Ir) alloys. The analysis is now going on to investigate the atomic scale miscibility and local structure of the alloys.

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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;Spin dynamics in the stripe-ordered buckled honeycomb lattice antiferromagnet Ba_2NiTeO_6, Magnetic excitations from the two-dimensional interpenetrating Cu framework in $Ba_2Cu_3O_4Cl_2$, Magnetic Structure and Dielectric State in the Multiferroic $Ca_2CoSi_2O_7$, A layered wide-gap oxyhalide semiconductor with an infinite ZnO_2 square planar sheet: $Sr_2ZnO_2Cl_2$, Magnetic metal-complex-conducting copolymer core-shell nanoassemblies for a single-drug anticancer platform, and Spin pseudogap in the S=1/2 chain material Sr_2CuO_3 with impurities.

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* Joint research among groups within ISSP.

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[†] Joint research with outside partners.

International MegaGauss Science Laboratory

Takeyama group

985 T close to 1000 T has been achieved by the electromagnetic flux compression megagauss generator. 1000 T-class electromagnetic flux compression megagauss generator is newly reconstructed and completed. A peak magnetic field of 400 T has been achieved with 1.3 MJ energy injection, showing high efficiency of the system. Magnetization measurement techniques are still in progress in the single-turn coil magagauss 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. Contactless ultra-high frequency AC-conductivity measurement techniques are developed and showed it is applicable to destructing short-pulse magnets of micro second pulse duration. The methods have been applied to investigate spin structures of frustrated magnetic materials, multiferro materials, and quantum spin systems, superconducting materials, and etc.

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2. †*Magnetization Process of the S = 1/2 Two-Leg Organic Spin-Ladder Compound BIP-BNO: K. Nomura, Y. H. Matsuda, Y. Narumi, K. Kindo, S. Takeyama, Y. Hosokoshi, T. Ono, N. Hasegawa, H. Suwa and S. Todo, J. Phys. Soc. Jpn. **86** (2017) 104713(1-3).

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Kindo group

We have succeeded in developing highly repetitive long pulse magnet. The magnet is used for the electric transport measurements and the heat capacity measurements. We have shortened the waiting time for cooling down the magnet to 1.5 hrs after generating the maximum field.

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5. †*Magnetization Process of the Kondo Insulator YbB_{12} 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).

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* Joint research among groups within ISSP.

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Tokunaga group

$BiFeO_3$ is perhaps the most extensively studied multiferroic material. Our highly accurate experiments of magnetostrsiction, magnetization, electric polarization in pulsed high magnetic fields revealed ferroelastic distortion in this material that can be controlled by magnetic field, and also emergence of novel magneto-electric phase at around room temperature. Theoretical calculation suggests a kind of conical spin order in this phase, which has a spin modulation vector normal to that in the cycloidal state at zero field. Change in the spin modulation vector is confirmed through neutron experiments.

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Y. Matsuda group

The phase diagram in B-T plain of solid oxygen has been constructed by several experiments including the optical transmission, magnetization, adiabatic heating effect, and magneto-caloric effect. The obtained phase diagram indicates that the field induced novel phase (θ phase) emerges from the α and β phases at low temperatures. The full magnetization curve of the organic S=1/2 spin ladder compound BIP-BNO is obtained using the single-turn coil megagauss field generator. A characteristic symmetric two-peak structure in dM/dB curve is a first experimental evidence that BIP-TENO is a prototypical organic (not containing magnetic ions) spin-ladder compound. High magnetic field property of the Kondo insulator YbB_{12} is also investigated by means of the magnetization. The second jump of the magnetization found around 102 T can correspond to the collapse of the Kondo bound state. It has been shown that the field-induced insulator-metal transition in YbB_{12} is interpreted as the energy gap closing by Zeeman effect without breaking the Kondo state. In addition to experiments on various materials, we have developed a technique for magnetostriction under ultrahigh magnetic fields in the range of 100 -1000 T.

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Kohama group

In 2017, our group upgrades the pulsed-field calorimeter for low temperature measurements of specific heat. With the new system, not only the accessibility to the low temperature, the sensitivity & accuracy of the C(T) data becomes compatible with

† Joint research with outside partners.

the C(T) data taken in steady fields. We also successfully developed new technique for measuring electric resistivity, which can operate in destructive pulsed field up to 120 T.

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Center of Computational Materials Science

Akai group

(1) L-edge resonant magneto-optical Kerr effect of Fe and Fe/Cu interfaces were calculated in the framework of KKR Green's function method and density functional theory. The results were compared with the recent experimentas performed by Matsuda's group of ISSP. (2) The method of first-principles calculation of the soft X-ray second harmonic generation (SHG) was developed. The SHG of $GaFeO_3$ was calculated by the method and the results were compared with the recent experiment performed by Matsuda's group of ISSP. (3) Maximum performance that might be expected for permanent magnet materials was estimated based on the density functional theory. The calculations concluded that the plausible upper limits of saturation magnetic polariza- tion, magnetic transition temperature, and the magnetocrystalline anisotropy constant of permanent magnet materials could be ~2.7 T, ~2000 K, and ~1000 MJm^{-3}, respectively. (4) We developed the method of calculating Seebeck coefficient in the framework of the Korringa–Kohn–Rostoker (KKR) method combined with the coherent potential approximation (CPA; KKR-CPA) and linear response theory. The main objective was to establish a practical first-principles scheme that can calculate the conductivities and Seebeck coefficients of metallic systems at finite temperature. Thus, it was necessary to include the effects of electron-phonon scattering, which plays a crucial role at finite temperature, particularly for ordered-structure systems where the conductivity diverges at T = 0 K. The approach combines three components: linear response theory in the framework of the KKR method; phonon calculations; and an alloy analogy applied to the local static phonons using the KKR-CPA. The calculated Cu resistivity and Seebeck coefficients for various transition- metal elements at finite temperature showed reasonably good overall agreement with experiment.

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Laser and Synchrotron Research Center

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* Joint research among groups within ISSP.

dence 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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I. Matsuda group

In 2017, we made large progress in developments of synchrotron radiation techniques at our beamline, SPring-8 BL07LSU. We succeeded in directly determining the complex permittivity tensor using a method combining a developed light source from a segmented cross undulator of synchrotron radiation and the magneto-optical Kerr effect. The empirical permittivity, which carries the electronic and magnetic information of a material, has element specificity and has perfect confirmation using the quantum-mechanical calculation for itinerant electrons systems. These results help in understanding the interaction of light and matter, and they provide an interesting approach to seek the best materials as optical elements, for example, in extended-ultraviolet lithographic technologies or in state-of-the-art laser technologies. Concerning the material science, we experimentally realized two-dimensional Dirac nodal line fermions in monolayer Cu_2Si. We also succeeded in capturing ultrafast carrier dynamics in massless and massive Dirac materials with high-harmonic generation lasers.

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* Joint research among groups within ISSP.

Kobayashi group

We are developing ultra-short and high-power laser system for photoemission spectroscopy and extreme light-matter interaction. We have started a study of a laser processing by using these lasers. High-rep rate and ultrashort lasers are also studied.

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14. NEDO 高輝度・高効率次世代レーザー技術開発プロジェクト：小林 洋平 , レーザー加工学会誌 24 **No.2** (2017) 1.

Itatani group

We built a high harmonic beamline for attosecond soft X-ray spectroscopy. The development was nearly completed, and attosecond soft-X-ray pulses around the carbon *K* edge (~284 eV) are routinely generated. We have also started to explore strong field phenomena in solids using intense mid-IR sources. We produced high harmonics of 5-μm light in GaSe crystals, and observed unusual behavior in polarization rotation. Photoemission experiments with a nanotip is expanded to a grating-like structures where we observe clear enhancement due to surface-propagating plasmons. Development of high-energy velocity map imaging apparatus was continued. Photoelectrons up to 1 keV were successfully imaged in the momentum space. Collaboration with Shin, Okazaki, and Matsuda groups was continued for time-resolved ARPES and Kerr-rotation experiments.

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Harada group

This year we have performed 17 collaborative works at BL07LSU HORNET endstation, four of which are related to the study on the behavior of water at various circumstances (water in plasma, water encapsulated in an electrolyte, hydrated water, and interfacial water). We also published four papers related to water. RIXS in operando conditions were frequently used for the study of fuel cell batteries and rechargeable Li- and Na-ion batteries. Angle (momentum) resolved system was also utilized for the oxygen analyses of strongly correlated systems like multi layered high Tc cuprate Bi2223 and other hole-doped cuprates, as well as for the soft X-ray inelastic diffraction (SXID) of $LaSrFeO_4$ more precisely taking the preliminary results of the previous year. For future studies on water related materials and SXID verification a liquid jet system was installed which removed the vacuum compatible membrane separating atmospheric pressure and high vacuum expecting more precise and quantitative analysis of the intensity of elastic scattering, which may also develop a new field that combines spectroscopy and diffraction in the soft X-ray region. Continuous studies on bio-inspired or bio-model compounds are ongoing, patiently and systematically controlling radiation damage problems and some of them (model compounds of Fe-S proteins, Mn cluster in photosystem II) have already been on the publication stage.

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Wadati group

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Kondo group

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Matsunaga group

Matsunaga group has started on July 2017 to investigate light-matter interactions and light-induced nonequilibrium phenomena in materials by utilizing terahertz wave, infrared, visible, and ultraviolet coherent light sources based on ultrafast pulsed laser technology. A stable mode-locked Ti:Sapphire oscillator with tunable bandwidth was installed for seed of an regenerative amplified laser system with pulse width less than 50 fs, which will be used as a source of ultrabroadband mid-infrared laser pulse. In addition, a compact diode-pump Yb:KGW femtosecond laser system was also installed for intense terahertz pulse generation. We developed conventional terahertz time-domain spectroscopy system and investigated terahertz electromagnetic response of quantum materials such as antiferromagnets fabricated by Nakatsuji group.

Okazaki group

We have investigated superconducting-gap structures of unconventional 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 2017, we have revealed superconducting gap anisotropy sensitive to nematic domains in FeSe, where it has been reported that time-reversal symmetry is broken around its nematic domain boundaries. In addition, we have found displacive-type excitation of coherent phonons in a parent compound of iron-based superconductors, $BaFe_2As_2$, and suggested a possibility that photo-induced superconductivity can be realized in this material.

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