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 2015 include: (1) Investigation by ^{31}P-NMR of the quasi two dimensional antiferromagnet $RbMoOPO_4Cl$ with the frustrating nearest neighbor and the next nearest neighbor interactions that lead to the identification of a stripe type antiferromagnetic order. (2) Combined studies of ^{7}Li-NMR and neutron scattering experiments on the breathing pyrochlore antiferromagnet $Li(Ga,In)Cr_4O_8$, in particular the observation of a second order phase transition in the In 5% doped sample. (3) Investigation of spin dynamics in the quantum spin ice compound $Pr_2Zr_2O_7$ by ^{91}Zr-NQR/NMR that revealed contrasting behavior when a magnetic field is applied along <001> and <111>.

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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 2015. (1) Field and temperature variations of the specific heat $C(H,T)$ of the heavy fermion superconductor URu_2Si_2 (T_c= 1.4 K) were examined at temperatures down to 200 mK. The occurrence of quasiparticle excitations due to the Doppler-shift effect was detected regardless of the field direction in $C(H)$, implying the presence of a line node. Furthermore, the polar-angle-dependence of the specific heat $C(\theta)$ under a rotating magnetic field within the *ac* plane exhibits a shoulder-like anomaly at $\theta \sim 45°$ and a sharp dip at $\theta = 90°$ (H // a) in the moderate-field region. These features are supported by theoretical analyses based on microscopic calculations assuming the gap symmetry of $k_z(k_x+ik_y)$, whose gap structure is characterized by a combination of a horizontal line node at the equator and point nodes at the poles. The present results have settled the previous controversy over the gap structure of URu_2Si_2 and have authenticated its chiral *d*-wave superconductivity. (2) We examined low-temperature magnetic properties of a new verdazyl radical crystal α-2-Cl-4-F-V. Molecular orbital calculations predict that this material is a spin-1/2 quasi-one-dimensional antiferromagnet. The magnetization curve at 0.1 K shows gapless behavior like conventional one-dimensional quantum spin systems and saturates at about 5 T. A peak is observed in the temperature dependence of the heat capacity at 0 T, indicating that a three-dimensional ordering occurs at about 0.2 K. On the other hand, the temperature dependence of the magnetization at various magnetic fields shows an anomaly similar to that observed in many of gapped spin systems. This behavior is attributed to the highly frustrated nature of the interchain interactions.

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Mori group

We have successfully developed and unvailed unprecedented functional properties for the molecular materials. The major achievements in 2015 are (1) to discover the peculiar hydrogen-bond-dynamics-based switching of conductivity and magnetism triggered by deuterium and charge transfers in the hydrogen-bond-unit for the purely organic conductor κ-D_3(Cat-EDT-ST)$_2$, (2) to develop the novel donor-acceptor-type molecular dyad with small HOMO-LUMO gap, and (3) to develop the chiral molecular conductors composed of chiral BEDT-TTF derivatives with hydrogen bonds, α'-[(*R*,*R*)-BEDT-TTF(CH_2OH)$_2$]$_2$$ClO_4$($H_2O$). The introduction of a large variety of molecule degree of freedom to solid promises the development of new trends in functional molecular materials.

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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 2015. (1) We discovered the first example of an antiferromagnet that exhibits the anomalous Hall effect at room temperature, the chiral antiferromagnet Mn_3Sn (2) The quantum criticality at ambient pressure in β-$YbAlB_4$ is found robust against pressure, and possibly forms a strange metal phase. In addition, this phase is separated from a magnetic criticality by a Fermi liquid phase stabilized under pressure (3) A field induced quantum metal-insulator transition was found in the pyrochlore iridate $Nd_2Ir_2O_7$, when the field is applied only along the narrow angle range close to [100]. (4) A Fermi node at the quadratic band touching in $Pr_2Ir_2O_7$ was found and indicates that $Pr_2Ir_2O_7$ should be viewed as a mother compound for various topological phases in the correlated electron system, such as Weyl semimetals, and topological insulators.

* Joint research among groups within ISSP.

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Division of Condensed Matter Theory

Takada group

Employing several standard techniques including the Green's-function method, quantum Monte Carlo simulations, band-structure calculations, and various types of variational approaches, we are studying several aspects of quantum many-body problems in condensed matter physics, based primarily on the first-principles Hamiltonian. This year we have studied the following issues: (1) The failure of the conventional self-consistent GW approximation in the calculation of both normal and superconducting properties is made clear by comparing the results among the G_0W_0 (one-shot GW), GW, and GWΓ approximations. (2) Diffusion Monte Carlo (DMC) simulations are performed on the system of an atom embedded in an electron gas with a view of investigating Kondo physics from first principles. A detailed analysis of the Friedel oscillations around the impurity atom

* Joint research among groups within ISSP.

reveals that a proton-embedded electron gas can exhibit the Kondo temperature well beyond 1000 K. The obtained accurate electron-density profile is used to improve 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. (3) With proposing a better functional form for the vertex function Γ, always satisfying both the Ward identity and the momentum conservation law, we study the low-density electron gas in the GWΓ scheme to find an anomalous mass reduction as a result of avoiding the collapse of the normal state into a spontaneously excited electron-hole pair condensed state. Concomitantly with this mass reduction, an anomalous behavior of the momentum distribution function is found for the density parameter r_s around 20.

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2. Generic Features of an Electron Injected into the Luttinger Liquid: H. Maebashi and Y. Takada, J. Supercond. Nov. Magn. **28** (2015) 1331-1335.

3. Role of the ward identity and relevance of the G^0W^0 approximation in normal and superconducting states: Y. Takada, Mol. Phys. **114** (2016) 1.

4. Theory for Reliable First-Principles Prediction of the Superconducting Transition Temperature: Y. Takada, in: *Carbon-based New Superconductors: Toward high-Tc superconductivity (ISBN 978-981-4303-30-9 (Hardcover), 978-981-4303-31-6 (eBook))*, Ch 8, edited by J. Haruyama, (Pan Stanford Publishing Pte. Ltd., 2015), pp. 193-230.

5. Reference Module in Materials Science and Materials Engineering: Y. Takada, in: *Materials Science and Materials Engineering*, edited by S. Mahfoudh and M. Nicholls, (Elsevier, 2016), B9780128035818007748.

Oshikawa group

We studied a wide range of fundamental problems in condensed matter theory and statistical mechanics. In particular, we discovered that even trivial phases, which are adiabatically connected to a product state without any entanglement, are not unique in the presence of an appropriate symmetry. We discussed a simple example of S = 1 quantum spin chain with a symmetry under a combined operation of the site-centered lattice inversion and the global π-rotation about z axis. In this model, there are two trivial phases, adiabatically connected to the Néel state and the large-D state (product of S^z=0 states), which are always separated by a quantum phase transition in the presence of the above symmetry. We demonstrated this using field theory, numerical calculation, and a general proof based on Matrix Product State representation. The present result brings about a new perspective in classification of quantum phases, a central issue in current condensed matter physics.

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2. †Selection of factorizable ground state in a frustrated spin tube: Order by disorder and hidden ferromagnetism: X. Plat, Y. Fuji, S. Capponi and P. Pujol, Phys. Rev. B **91** (2015) 064411 (1-21).

3. †Spin fluctuations and superconductivity in layered f-electron superlattices: Y. Tada and R. Peters, Phys. Rev. B **92** (2015) 035129(1-8).

4. †Absence of Quantum Time Crystals: H. Watanabe and M. Oshikawa, Phys. Rev. Lett. **114** (2015) 251603(1-5).

5. †Distinct Trivial Phases Protected by a Point-Group Symmetry in Quantum Spin Chains: Y. Fuji, F. Pollmann and M. Oshikawa, Phys. Rev. Lett. **114** (2015) 177204.

6. Gravitational Casimir Effect: J. Q. Quach, Phys. Rev. Lett. **114** (2015) 081104(1-5).

7. †Orbital Angular Momentum and Spectral Flow in Two-Dimensional Chiral Superfluids: Y. Tada, W. Nie and M. Oshikawa, Phys. Rev. Lett. **114** (2015) 195301.

8. 「物性物理学」〜物質に潜む普遍的概念〜：押川 正毅 , 数理科学 **620** (2015) 40-45.

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† Joint research with outside partners.

12. †Plaquette order in the SU(6) Heisenberg model on the honeycomb lattice: P. Nataf, M. Lajkó, P. Corboz, A. M. Läuchli, K. Penc and F. Mila, Phys. Rev. B **93** (2016) 201113(R)(1-6).

13. Spin gravitational resonance and graviton detection: J. Q. Quach, Physical Review D **93** (2016) 104048(1-6).

14. † ウラン系強磁性超伝導における強磁性ゆらぎが誘起するスピン三重項超伝導 : 石田 憲二 , 服部 泰佑 , 佐藤 憲昭 , 出口 和彦 , 多田 靖啓 , 藤本 聡 , 固体物理 **50** (2015) 123-132.

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Tsunetsugu group

We have studied optical conductivity near an antiferromagnetic phase transition in the square-lattice Hubbard model at half filling using the cluster dynamical-mean field approach. We investigated the effects of vertex corrections on optical conductivity and found that they have large contributions and change some important features of optical conductivity. The vertex corrections enhance frequency dependence of conductivity in both metallic and insulating phaes. Another important discovery is the presence of a temperature region above the transition temperature where dc conductivity shows non-increasing behavior with lowering temperature. This is not due to a pseudogap behavior, but the electron spectral function does not show a dip at Fermi energy. (Reference: arXiv:1605.00387) We have continued the study of quadrupole order in Pr 1-2-20 system. We used a classical Monte Carlo calculation to investigate the effects of thermal fluctuations in temperature-magnetic field phase diagram. We found that the same number of ordered phases appear as predicted by our previous mean-field analysis, but the phase boundaries are strongly modified by thermal fluctuations and have a different topology. A new tetracritical point appears when magnetic field is applied along (001) direction. Criticality of parasitic ferro quadrupole order is also investigated, and we have found an unusual critical behavior in their temperature dependence. (Reference arXiv:1605.05175) We have also studied an antiferromagnetic Heisenberg model on breathing pyrochlore lattice, and found that the ground state in the S = 3/2 case has an interesting "dimerized" pattern that differs from the previously studied S = 1/2 case.

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2. Dynamical Characteristics of the Mott Transition: Examination of Doublon Dynamics in a Triangular-lattice Hubbard Model: T. Sato and H. Tsunetsugu, Physics Procedia **75** (2015) 376-382.

Sugino group

We have done first-principles study of the excited-states, ferroelectric interfaces, electrochemical interfaces, and the ground-state wavefunctions. We have improved our GW+ BSE program of excited-state calculation so as to manipulate large number of atoms (~200 atoms), which has significantly activated collaboration with experiments. We also advanced density functional methods to compute the electrically biased interface, which are used to investigate the system of negative capacitance as well as the electrochemical reactions. We further developed a variational approach to strongly correlated electron systems to investigate the structure of the many-body wavefunction.

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4. Configuration interaction with antisymmetrized geminal powers: W. Uemura, S. Kasamatsu and O. Sugino, Phys. Rev. A **91** (2015) 062504.

5. *Vibronic Structures in Absorption and Fluorescence Spectra of Firefly Oxyluciferin in Aqueous Solutions: M. Hiyama, Y. Noguchi, H. Akiyama, K. Yamada and N. Koga, Photochem. Photobiol. **91** (2015) 819.

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* Joint research among groups within ISSP.

8. *Pressure dependence of the magnetic ground states in MnP: M. Matsuda, F. Ye, S. E. Dissanayake, J. -G. Cheng, S. Chi, J. Ma, H. D. Zhou, J. -Q. Yan, S. Kasamatsu, O. Sugino, T. Kato, K. Matsubayashi, T. Okada and Y. Uwatoko, Phys. Rev. B **93** (2016) 100405(1-5).

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Kato group

The main research subject of our laboratory is theory of non-equilibrium properties in nanoscale devices. We have studied (1) photon-assisted current noises under strong AC fields in quantum dot systems, (2) a multi-orbital Anderson impurity at high bias voltages, and (3) non-equilibrium current noises of quantum dots in the Kondo regime. We have also studied form factors of the Kondo model by the Bethe ansatz method.

1. Effects of Coulomb interaction on photon-assisted current noise through a quantum dot: T. J. Suzuki and T. Kato, Phys. Rev. B **91** (2015) 165302(1-12).

2. Exact Green's function for a multiorbital Anderson impurity at high bias voltages: A. Oguri and R. Sakano, Phys. Rev. B **91** (2015) 115429(1-14).

3. Universality of non-equilibrium fluctuations in strongly correlated quantum liquids: M. Ferrier, T. Arakawa, T. Hata, R. Fujiwara, R. Delagrange, R. Weil, R. Deblock, R. Sakano, A. Oguri and K. Kobayashi, Nature Phys. **12** (2015) 230-235.

Division of Nanoscale Science

Iye group

Electronic transport in monolayer graphene grown on vicinal surface of 6H-SiC(0001) with a quasi-regular step-and-terrace structure is studied. Conductivity under a magnetic field normal to the plane showed a high degree of anisotropy. The quantum Hall effect (QHE) with zero resistance manifests itself for the current along the steps, whereas the QHE is obscured by pronounced positive magnetoresistance with quadratic magnetic-field dependence for the current across the steps.

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Katsumoto group

Conductance fluctuation in InAs two-dimensional electrons versus in-plane magnetic field was found and attributed to the sign of so called "Zitterbewegung" (trembling motion) due to spin-orbit coupling. We have succeeded in making low resistance semiconductor-superconductor junctions not only for InAs two-dimensional electrons but also for a diluted magnetic semiconductor (In,Fe)As. Anomalous response in the latter will be our next subject.

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Otani group

We have studied on three topics including spin Hall effect, spin diffusion length, and magnonic crystals.

1. Tunable configurational anisotropy in collective magnetization dynamics of $Ni_{80}Fe_{20}$ nanodot arrays with varying dot shapes: B. K. Mahato, S. Choudhury, R. Mandal, S. Barman, Y. Otani and A. Barman, J. Appl. Phys. **117** (2015) 213909.

2. Tunable spin wave spectra in two-dimensional $Ni_{80}Fe_{20}$ antidot lattices with varying lattice symmetry: R. Mandal, S. Barman, S. Saha, Y. Otani and A. Barman, J. Appl. Phys. **118** (2015) 053910.

3. Crossover between spin swapping and Hall effect in disordered systems: H. B. M. Saidaoui, Y. Otani and A. Manchon, Phys. Rev. B **92** (2015) 024417.

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5. Spin relaxation mechanism in a highly doped organic polymer film: M. Kimata, D. Nozaki, Y. Niimi, H. Tajima and Y. Otani, Phys. Rev. B **91** (2015) 224422.

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8. Spin relaxation characteristics in Ag nanowire covered with various oxides: S. Karube, H. Idzuchi, K. Kondou, Y. Fukuma and Y. Otani, Appl. Phys. Lett. **107** (2015) 122406.

9. Selective mode excitation in three-chained magnetic vortices: N. Hasegawa, S. Sugimoto, H. Fujimori, K. Kondou, Y. Niimi and Y. Otani, Appl. Phys. Express **8** (2015) 063005-1.

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11. Spin transport in non-magnetic nano-structures induced by non-local spin injection: H. Idzuchi, Y. Fukuma and Y. Otani, Physica E: Low-dimensional Systems and Nanostructures **68** (2015) 239.

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Komori group

Reproducible dependence of the STM images on the distance between the surface and the STM tip apex for a monatomic layer of iron nitride (Fe_2N) formed on a Cu(001) surface was found in the bias-voltage range corresponding to the Fe 3*d* states. The results are attributed to a shift in surface orbitals detected by the tip from the *d* states to the *sp* states. Electronic structures of the Pt-adsorbed Ge(001) surface with a one-dimensional atomic structure were studied by high-resolution ARPES and SARPES. One-dimensional Fermi surfaces of four surface states were confirmed by ARPES. One of them is spin-split due to the Rashba effect.

1. †Nonlinear terahertz field-induced carrier dynamics in photoexcited epitaxial monolayer graphene: H. A. Hafez, I. Al-Naib, M. M. Dignam, Y. Sekine, K. Oguri, F. Blanchard, D. G. Cooke, S. Tanaka, F. Komori, H. Hibino and T. Ozaki, Phys. Rev. B **91** (2015) 035422 (1-9).

2. *Scanning tunneling spectroscopy study of quasiparticle interference on dual topological insulator $Bi_{1-x}Sb_x$: S. Yoshizawa, F. Nakamura, A. A. Taskin, T. Iimori, K. Nakatsuji, I. Matsuda, Y. Ando and F. Komori, Phys. Rev. B **91** (2015) 045423(1-6).

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6. †*Selective Formation of Zigzag Edges in Graphene Cracks: M. Fujihara, R. Inoue, R. Kurita, T. Taniuchi, Y. Motoyui, S. Shin, F. Komori, Y. Maniwa, H. Shinohara and Y. Miyata, ACS Nano **9** (2015) 9027-9033.

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

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Yoshinobu group

We conducted several research projects in the fiscal year 2015. (1) The activation and hydrogenation of CO_2 on clean and Zn-deposited Cu(111) and Cu(997) surfaces studied by AP-XPS. (2) The surface chemistry of formic acid on Zn-Cu(111) studied by SR-PES. (3) Spectroscopic characterization of H-Cu(111), Zn-Cu(111) and Pd-Cu surfaces by XPS. (4) Spectroscopic characterization of Au on $SrTiO_3$ under O_2 exposure using SR-XPS (5) LT-STM study of CO_2 on Cu(997) (6) Independently driven four-probe conductivity measurement of organic thin films.

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2. Observation of Fano line shapes in infrared vibrational spectra of CO_2 adsorbed on Cu(997): T. Koitaya, Y. Shiozawa, K. Mukai, S. Yoshimoto and J. Yoshinobu, J. Chem. Phys. **144** (2016) 054703.

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4. [*]Real-time observation of reaction processes of CO_2 on Cu(997) by ambient-pressure X-ray photoelectron spectroscopy: T. Koitaya, S. Yamamoto, Y. Shiozawa, K. Takeuchi, R.-Y. Liu, K. Mukai, S. Yoshimoto, K. Akikubo, I. Matsuda and J. Yoshinobu, Topic in Catalysis **59** (2016) 526-531.

5. The chemistry of simple alkene molecules on Si(100)c(4x2): the mechanism of cycloaddition and their selectivities: K. Akagi and J. Yoshinobu, Surface Science (2016), accepted for publication.

Hasegawa group

We have developed spin-polarized scanning tunneling microscopy (SP-STM), which enables us to detect the orientation of spins / magnetic moments on surfaces in atomic-scale spatial resolutions. Using the method, we investigated the formation mechanism of spin spiral structures of Mn ultrathin films formed on a W(110) substrate. Because of the absence of inversion symmetry due to the thin film structure and the spin-orbit interaction in the heavy-elemental substrate, the Dzyaloshinskii-Moriya interaction (DMI) is exerted among the spins in the thin films, which induces chirality in the spin structures. In order to investigate the details of DMI, we directly measured the rotational sense of the spin spiral structures by SP-STM, and revealed that both 1st and 2nd Mn layers exhibit chirality and the same polarization of DMI despite their different types of spin structures and propagation directions. These results, combined with previous reports on the chirality of domain walls observed in magnetic thin films on the same substrate, lead us to conclude that the DMI polarization is dominantly determined by the substrate. Aiming for a bottom-up approach of fabricating quantum spin systems and their microscopic investigations, we studied the adsorption of oxygen molecules, which have a spin triplet state (S = 1) as a ground state, on a Ag(111) substrate. It was found that by low temperature exposure the molecules adsorb on the substrate in a physisorbed manner lying down to form a triangular

[†] Joint research with outside partners.

lattice. Different from an isosceles triangular lattice expected from the ellipsoidal shape of the molecule, the lattice is deformed to scalene. Based on a Monte Carlo calculation using parameters that account for the solid oxygen phases, we found that the introduction of antiferromagnetic interaction among the adsorbed molecules explain the deformation quantitatively. The antiferromagnetic order indicates the preservation of the spin of the adsorbed molecules, opening up the possibility that the system can be utilized for fabrication / construction of one- or two- dimensional spin structures using an atom / molecular manipulation method of STM.

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7. Insensitivity of atomic point contact conductance to a moiré structure: H. Kim and Y. Hasegawa, Phys. Rev. B **93** (2016) 075409(1-6).

8. Spatial variation in local work function as an origin of moiré contrast in scanning tunneling microscopy images of Pb thin films / Si(111): H. Kim and Y. Hasegawa, Jpn. J. Appl. Phys. (2016), accepted for publication.

9. Superconducting proximity effect on Rashba-split Pb/Ge(111)-$\beta\sqrt{3} \times \sqrt{3}$ surface: H. Kim, Y. Miyata and Y. Hasegawa, Supercond. Sci. Technol. (2016), accepted for publication.

Lippmaa group

We work on various aspects of oxide thin films and interfaces. One of our aims is to explore novels polar oxide phases that may exhibit new type of magnetoelectric coupling. In particular, we have looked at double perovskites that can sustain both ferromagnetism and ferroelectricity in a strained lattice. We have continued working on magnetic interfaces, mostly looking at band alignment and magnetic coupling in manganite-titanate heterostructures. The third topic is the development of photocatalytic materials. Our recent work has involved the analysis of carrier dynamics in optically excited crystals, surface chemical reactions, and the development of nanoscale composite materials for efficient collection of photogenerated charge in a photocatalyst.

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Division of Physics in Extreme Conditions

Uwatoko group

We report electrical resistivity, ac magnetic susceptibility and X-ray absorption spectroscopy measurements of intermediate valence $YbNi_3Ga_9$ under pressure and magnetic field. We have revealed a characteristic pressure-induced Yb valence crossover within the temperature-pressure phase diagram, and a first-order metamagnetic transition is found below P_c ~9 GPa where the system undergoes a pressure-induced antiferromagnetic transition. Zirconium-based bulk metallic glass (Zr-based BMG) has outstanding properties as a cylinder material for piston-cylinder high pressure apparatuses and is especially useful for neutron scattering. The piston cylinder consisting of a Zr-based BMG cylinder with outer/inner diameters of 8.8/2.5 mm sustains pressures up to 1.81 GPa and ruptured at 2.0 GPa, with pressure values determined by the superconducting temperature of lead. We report the discovery of pressure-induced superconductivity below T_c = 14 K in the iron-based spin-ladder material $BaFe_2S_3$, a Mott insulator with striped-type magnetic ordering below ~120 K. Our findings indicate that iron-based ladder compounds represent promising material platforms, in particular for studying the fundamentals of iron-based superconductivity. The perovskite $PbCrO_3$ is an antiferromagnetic insulator. However, the fundamental interactions leading to the insulating state in this single valent perovskite are unclear. We report a variety of insitu pressure measurements including electron transport properties, X-ray absorption spectrum, and crystal structure study by X-ray and neutron diffraction. These studies reveal key information leading to the elucidation of the physics behind the insulating state and the pressure-induced transition.

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[*] Joint research among groups within ISSP.

Osada group

We have systematically studied quantum Hall transport in monolayer-bilayer graphene heterojunctions on hexagonal boron nitride substrate. It has been found that the observed asymmetric transverse and Hall resistances across the junction are well understood by the Landauer-Büttiker edge transport picture assuming the pair annihilation of edge channels with opposite chirality at the junction. We show that the above picture works well even in the system where the monolayer and bilayer regions have different carrier density, which corresponds to the preceding work. This result demonstrates the bulk-edge correspondence at the boundary of two quantum Hall states on different crystal and band structures. In addition, we found that fine structures around charge neutrality points, which are considered to originate from the degeneracy breaking of zero-energy Landau levels of monolayer and bilayer graphene.

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Yamashita group

As a joint project with Dr. Shishido at Osaka Prefecture University, we've performed dHvA measurements of the heavy-fermion superconductor $CeCoIn_5$. We succeeded to measure clear quantum oscillation measurements of the alpha bands of $CeCoIn_5$ down to 5 mK and up to 10 T. Unexpectedly, we found that the amplitude of the quantum oscillation is suppressed below 20 mK at 8 T (above H_{c2} of $CeCoIn_5$). At the same time, the frequency of the quantum oscillation shows a drop. These changes can be attributed to an emergence of a new ordered phase neighboring the superconducting phase. To clarify the property of the new phase, we started NMR measurements of $CeCoIn_5$ at ultra-low temperatures with Takigawa group, which is still a project under way in 2016. We've also measured longitudinal and transverse thermal transport measurements of a candidate material of quantum spin liquid, $Ba_3CuSb_2O_9$. We found that the longitudinal thermal conductivity is strongly suppressed in wide temperature range, showing that there are strong scatters of phonons. Further, a clear thermal Hall effect has been observed. Given that there are no mobile spin excitations in $Ba_3CuSb_2O_9$ from our measurements and NMR measurements, this thermal Hall effect is a phonon Hall effect. We believe that this work is the first systematic study of a thermal Hall effect of phonons including the temperature dependence of the thermal Hall conductivity. We've performed thermal Hall measurements of Mn_3Sn where the first observation of the anomalous Hall effect in antiferromagnetic system has been reported. A clear anomalous thermal Hall effect has been observed. We found that the temperature dependence of the Lorentz number implies that intrinsic scatterings play an important role for the anomalous Hall effect.

Materials Design and Characterization Laboratory

Hiroi group

One-Third Magnetization Plateau with a Preceding Novel Phase is discovered in Volborthite. We have synthesized high-quality single crystals of volborthite, and carried out high-field magnetization measurements up to 74 T and ^{51}V NMR measurements up to 30 T. An extremely wide 1/3 magnetization plateau appears above 28 T and continues over 74 T at 1.4 K, which has not been observed in previous studies using polycrystalline samples. NMR spectra reveal an incommensurate order (most likely a spin-density wave order) below 22 T and a simple spin structure in the plateau phase. Moreover, a novel intermediate phase is found between 23 and 26 T, where the magnetization varies linearly with magnetic field and the NMR spectra indicate an inhomogeneous distribution of the internal magnetic field. This sequence of phases in volborthite bears a striking similarity to those of frustrated spin chains with a ferromagnetic nearest-neighbor coupling J_1 competing with an antiferromagnetic next-nearest-neighbor coupling J_2. In addition, the metal-insulator transition (MIT) of VO_2 is discussed with particular emphasis on the structural instability of the rutile compounds toward dimerization. Ti substitution experiments reveal that the MIT is robust up to 20% Ti substitutions and occurs even in extremely thin V-rich lamellas in spinodally decomposed TiO_2-VO_2 composites, indicating that the MIT is insensitive to hole doping and essentially takes on a local character. These observations suggest that either electron correlation in the Mott-Hubbard sense or Peierls (Fermi-surface) instability plays a minor role on the MIT. Through a broad perspective of crystal chemistry on the rutile-related compounds, it is noted that VO_2 and another MIT compound NbO_2 in the family eventually lie just near the borderline between the two structural groups with the regular rutile structure and the distorted structures characterized by the formation of dimers with direct metal-metal bonding. It is also shown that the two compounds of the rutile form do not follow the general trends in structure observed for the other rutile compounds, giving clear evidence of an inherent structural instability present in the two compounds. The MITs of VO_2 and NbO_2 are natural consequences of structural transitions between the two groups, as all the d electrons are trapped in the bonding molecular

† Joint research with outside partners.

orbitals of dimers at low temperatures. Such dimer crystals are ubiquitously found in early transition metal compounds having chain-like structures, such as $MoBr_3$, $NbCl_4$, Ti_4O_7, and V_4O_7, the latter two of which also exhibit MITs probably of the same origin. In a broader sense, the dimer crystal is a kind of "molecular orbital crystals" in which virtual molecules made of transition metal atoms with partially-filled t_{2g} shells, such as dimers, trimers or larger ones, are generated by metal-metal bonding and are embedded into edge- or face-sharing octahedron networks of various kinds. The molecular orbital crystallization opens a natural route to stabilization of unpaired t_{2g} electrons in crystals.

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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 2015 include: (1) new interpretations and findings of computational results for the SU(N) Heisenberg models with and without higher order interactions, (2) development of quantum Monte Carlo code for Bose systems in continuous media, (3) correlation between computational hardness of the spin glass instances and the thermodynamic properties and (3) large-scale non-equilibrium molecular dynamics simulation of bubble growth in under-pressured near-transition liquid.

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Noguchi group

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Materials Synthesis and Characterization group

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† Joint research with outside partners.

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), 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 2015 include (1) development of high-toughness Ion gel for CO_2 separation, (2) gelation and cross-link inhomogeneity of phenolic resins, (3) structure evolution of catalyst ink for fuel cell in drying process, (4) rubber elasticity for percolation network consisting of Gaussian chains, (5) gelation mechanism of Tetra-Armed Poly(ethylene glycol) in aprotic ionic liquid, (6) structural analysis of lipophilic polyelectrolyte solutions and gels in low-polar solvents and so on.

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Yoshizawa group

A systematic study on spin dynamics in a two-dimensional transition-metal Ni oxide has been carried out with use of the high resolution chopper spectrometer installed at BL12 in the Material and Life Science Facility, J-PARC. The checkerboard-type spin-charge ordering in the highly hole-doped region of the layered nickelate was studied in detail. The nature of the excitation spectra and the thermodynamic properties in the checkerboard phase was found to show qualitative differences from those in the stripe phase. Magnetic properties of a family of Ce-based non-centrosymmetric heavy fermion compounds $CeTSi_3$ (T=transition metal ions) were also studied.

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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, we have succeeded to observe the inelastic neutron scattering spectra of palladium hydride nanoparticles. The peaks characteristic to the nanoparticles are attributed to the vibration of the H atoms located at the tetrahedral sites of the Pd lattice, which were predicted by our neutron powder diffraction work. Another topic is on the dynamics of a reverse osmotic membrane consisting of aromatic polyamide and water. This system is remarked for seawater desalination and waste-water reclamation. Several quasielastic neutron scattering experiments in a wide time range (0.5 ps to 5 ns) revealed that the polyamide network is drastically plasticized by water and moving with water even at 240 K. This information will give a new insight into the mechanism of water purification. Other than above topics, we have made some progresses in the studies on vapor-deposited molecular glasses and ionic liquids with plastically crystalline phases.

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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; complex magnetostructural order in the frustrated spinel $LiInCr_4O_8$, magnetic model in multiferroic $NdFe_3(BO_3)_4$, specific heats of triangular spin tube in magnetic fields, and magnetic anti-cancer compound for magnet-guided delivery and magnetic resonance imaging.

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International MegaGauss Science Laboratory

Takeyama group

Single-walled carbon nanotubes (SWNT) with a typical tube diameter an order of 1 nm are characterized by the quasi-one dimensional system. Optical properties are enriched by the enhancement of the excitonic band-edge structure. When a magnetic flux penetrates through the tube, the electronic band structure is subjected to substantial modulation via the mechanism of Aharonov-Bohm (A-B) effect. This effect lifts the quantum degeneracy of the band-edge states, induces splittings of the exciton optical absorption peak in megagauss magnetic field. The magneto-optical A-B splitting was investigated in magnetic fields of up to 300 – 400 T by observing band-edge exciton absorption spectra. The spectra evolved as a simple bright and dark exciton splitting with a linear magnetic field dependence as has been predicted by T. Ando. The ratio of the splitting is governed by a microscopic information of the environment dielectric substances surrounding the SWNTs.

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Kindo group

Long pulsed magnetic field has been improved. The maximum field of long pulse magnet was limited to 36 T due to the control system. We have improved the control system and succeeded in generating 42.5 T. The other improvement is development of almost perfect flat-top field. We have added a small coil into the bore of the large long pulse magnet and controlled the small coil to obtain the flat-top magnetic field. We have succeeded in generating 40 ± 0.005 T for 0.2 sec. These improvements will expand the possibility of the high field study on the condensed matter physics.

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Tokunaga group

We are focusing on physics in the quantum limit state, in which all the carriers are accommodated in the lowest Landau level. Since the carriers are confined in the smallest cyclotron orbit, kinetic degree of freedom normal to the field is suppressed. Thereby, the ratio between Coulomb interaction and bandwidth becomes large. Such strong correlation in the quantum limit state can realize anomalous quantum state. We can realize the quantum limit state in some kinds of semimetals with using non-destructive pulse magnets installed at ISSP. We studied magnetization and transport properties on various types of graphite in pulsed magnetic fields up to 74 T. The results suggest that the quantum limit state is realized in magnetic fields greater than 53 T applied along the *c*-axis. From systematic experimental studies, we proposed emergence of excitonic BCS-like state in

[*] Joint research among groups within ISSP.

the quantum limit state of graphite. We also studied transport properties of the semimetallic black phosphorus under pressure. We found anomalously large positive magnetoresistance and quantum oscillations in this material. The observed small Fermi surfaces, high mobilities, and light effective masses of carriers in semimetallic black phosphorus are comparable to those in the representative elemental semimetals of bismuth and graphite.

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Y. Matsuda group

The valence state and magnetization of the heavy fermion compound α-$YbAlB_4$ have been investigated. This compound shows the strong valence fluctuation and its Yb valence is around 2.8 which is distinctly smaller than the expected valence state 3.0 for local magnetic Yb ions. Although the fluctuated valence is expected to be influenced by magnetic field due to the suppression of the Kondo effect, the valence state has been found to be almost independent of magnetic field even at rather high magnetic field of up to 40 T. This experimental fact contrasts to that obtained in a related antiferomagnetic compound α-$YbAl_{1-x}Fe_xB_4$ (x = 0.115); the small valence increase is observed when magnetic field exceeds 20 T. The quantum criticality might be

† Joint research with outside partners.

enhanced in $YbAlB_4$ at low temperatures and the criticality is not significant in Fe-doped substance, which may explain the different magnetic field dependence of the Yb valence. In addition to the study of $YbAlB_4$, the B-T phase diagram of solid oxygen has been clarified and the high-field θ-phase has found to have low entropy and be clearly different from the high-tempereture γ-phase. We also studied issulator-metal transtion of Co-oxides, Fe-based superconductors and magneto-optics of the multiferroic CuB_2O_4.

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Center of Computational Materials Science

Akai group

(1) It is crucial to treat f-states properly to describe the magnetic properties of rear-earth permanent magnet materials. However, the local or semi-local approximations to the density functional method, which is the common basis of first-principles electronic structure calculations, are unable to treat the f-states in a reasonable way. To overcome this situation we have developed several methods that go beyond the local density approximation. One of them are the optimized effective potential method combined with the exact-excahnge and random-phaseapproximation. Another is the self-interaction corrected LDA/GGA applied to f-states. Using these methods, the magnetic crystalline anisotropy of $Sm_2Fe_{17}N_x$ ($0<x<3$) is calculated. The results obtained by two different methods show considerable differences and the origin of these discrepancies are discussed. (2) A scheme that combines the non-equilibrium Green's function method with the Korringa-Kohn-Rostoker (KKR) Green's function method is proposed. The scheme applied to Schottky contact composed of Al/GaN/Al trilayer. The transport property of this system under various finite bias voltages is calculated. It is shown that the asymmetric behavior of electron transport against the direction of bias voltage occurs in this system, confirming the feature of rectification.

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Ozaki Taisuke group

First-principles calculations based on density functional theories (DFT) have been playing an invaluable role as a cornerstone in computational materials science. For a wide variety of materials ranging from metals, insulators, semiconductors, and molecules the DFT calculations enable us to quantitatively predict the chemical and physical properties within a reasonable computational cost. With a recent advance of massively parallel computers, even realistic materials discussed in industrial fields have been becoming the potential targets. However, it is a challenging problem to develop algorithms and software being suitable for massively parallel computers typified by the K-computer, which results in a fact that users and developers are distinguished from each other in recent years, and that most of users use specific software. We have been developing OpenMX (Open source package for Material eXplore) towards a de fact standard DFT code, and in 2015 released the Ver. 3.8 to the public under GNU-GPL. To improve numerical accuracy, optimized pseudopotentials and pseudo-atomic basis functions have been developed based on a norm-conserving pseudopotential method with multiple reference energies and a variational optimization method for radial basis functions. The optimization over 80 elements in the periodic table results in the reliable database storing optimized pseudopotentials and pseudo-atomic basis functions, where the accuracy of the database was validated by the delta gauge method. In addition, new functionalities including stress tensor calculation, band unfolding method, and eigenchannel/real space current analysis have been developed, which makes OpenMX a versatile tool for many applications.

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Laser and Synchrotron Research Center

Suemoto group

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† Joint research with outside partners.

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Shin group

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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, we have succeeded in realizing fast-switching (10 Hz) of the light polarizations for the segmented cross-type undulator. Moreover, we could measure a spectrum of X-ray magnetic circular dichroism for a magnetic sample using the fast-switching of left and right circular polarized light. At the end-station, we routinely supported picosecond-time-resolved SX photoemission spectroscopy experiments of joint-researches. Studies of photovoltaics and photocatalysis have been carried out mainly. In the laboratory, we studied electronic structure of novel two-dimensional materials that could show intriguing dynamical properties.

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Kobayashi group

We have demonstrated the highest repetition rate in a Kerr-lens mode-locked oscillator in the world. 15-GHz mode space of the optical frequency comb can be resolved by using commercially available spectrum analyzer. We started to develop a new HHG beam line for industrial applications. We have demonstrated 300-mW, 193-nm light source with single longitudinal mode at 6 kHz repetition rate for next generation lithography technology.

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* Joint research among groups within ISSP.

Itatani group

We carried out several application experiments using the optical parametric chirped pulse amplification (OPCPA) system that can produce carrier-envelope phase (CEP)-stable, 1.5-mJ, 10-fs infrared pulses at a repetition rate of 1 kHz. First, we produced soft-X-ray continuum extending to the photon energy of 320 eV, and measured the static absorption spectrum of a thin film containing carbon atoms. We successfully resolved the peaks arising from the C=C and C-C bonding with an accumulation time of approximately 100 seconds. This result shows the capability of laser-based time-resolved soft-X-ray absorption spectroscopy. Second, we measured the photoelectron spectra of ionizing atoms, and observed the CEP-dependent high-energy structures. By mapping the CEP-dependent cutoffs of photoelectron spectra, we successfully reproduced the differential cross sections of rare gas atoms with a high degree of agreement with the most advanced scattering theory. Third, under the collaboration with Prof. Tanaka at Kyoto University, we produced broadband THz pulses using organic crystals. New directions of the BIBO-based ultrabroadband optical parametric amplifiers are pursuit as well. First, we developed a high-repetition-rate optical parametric amplifier using newly developed dispersion compensation mirrors. We have successfully produced CEP-stable 10 uJ, 9-fs infrared pulses at 20 kHz, which were applied to high-throughput electron scattering experiments. Second, we modified a high-energy OPCPA system to amplify two spectral components in infrared followed by differential frequency generation, resulting in the generation of intense mid-infrared pulses. A strong optical field up to 50 MV/cm was achieved with a capability of sub-cycle EO sampling using 6.5-fs visible pulses. We also kept collaboration with Shin, Komori, and Matsuda groups at LASOR-ISSP on time-resolved ARPES using a femtosecond EUV source. Photo-induced electronic dynamics of $CuM_{0.17}Bi_2Se_3$ and graphene are successfully measured.

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Harada group

After three years development of differential pumping system we have for the first time succeeded in the near ambient pressure soft X-ray RIXS experiments at SPring-8 BL07LSU. The best demonstration was done for O 1*s* RIXS of SiO_2 under around 360 Torr (0.5 bar) air pressure. We also have implemented rotation of the RIXS spectrometer to enable momentum dependent RIXS experiments urgently requested for the study of strongly correlated systems. This year we have accepted 8 collaborative works at BL07LSU HORNET endstation, which include oxygen site analysis of high Tc cuprates, operando analysis of Li ion battery electrodes, RIXS study of multiferroic materials applying magnetic field, spin transition of $LaCoO_3$, monitoring vibrational excitations at Ti site in ferroelectric $BaTiO_3$, and electronic structure analysis of high concentration electrolyte for Li ion batteries.

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Wadati group

We succeeded in the observation of a devil's staircase in the novel spin-valve system $SrCo_6O_{11}$ by resonant soft x-ray scattering. We also performed time-resolved reflectivity study of ferrimagnetic alloy GdFeCo thin films by using seeded free electron laser in FERMI (Italy), and observed ultrafast spin-switching of Fe spins by resonant magneto-optical Kerr effect.

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Kondo group

We use angle-resolved photoemission spectroscopy (ARPES) with ultrahigh energy resolution. The main findings in 2015 are as follows: (1) Quadratic Fermi Node in a 3D Strongly Correlated Semimetal. (2) Point nodes persisting far beyond Tc in Bi2212.

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Okazaki group

We have developed and improved a time- and angle-resolved photoemission (TrARPES) apparatus using EUV and SX lasers by high harmonics generation (HHG). In the fiscal year 2015, we have installed a new Ti:Sapphire regenerative amplifier system and fairly improved a performance and stability of this apparatus. We have studied nonequilibrium electronic states of semiconductor surfaces, graphene, high-Tc cuprates, iron-based superconductors, and strongly correlated electron systems. Particularly, we have observed coherent phonon excitations both in the hole and electron Fermi surfaces of a parent compound of iron-based superconductors $BaFe_2As_2$. In addition, we have also investigated superconducting-gap structures of iron-based superconductors and BiS2-based superconductors by a low-temperature and high-resolution laser ARPES apparatus.

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