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 2020 include: (1) development of systematic methods to identify symmetries of ordered phases with electronic multipoles from the angle dependence of the NMR Knight shift and their application to ^{111}Cd-NMR measurements in the spin-orbit coupled metallic pyrochlore compound $Cd_2Re_2O_7$, (2) quantitative determination of magnetic-field-induced dipolar and octupolar moments in the low-temperature ordered phases of the 5*d* double-perovskite oxide Ba_2MgReO_6 based on the ^{17}O NMR experiments. In this material, strong spin-orbit coupling combined with the cubic crystal field generates a quartet ground state with $J_{\rm eff} = 3/2$, providing ideal platform to explore multipolar order of t_{2g} electron systems.

1. *Field-Orientation Effect on Ferro-Quadrupole Order in $PrTi_2Al_{20}$: S. Kittaka, T. Taniguchi, K. Hattori, S. Nakamura, T. Sakakibara, M. Takigawa, M. Tsujimoto, A. Sakai, Y. Matsumoto and S. Nakatsuji, J. Phys. Soc. Jpn. **89**, 043701(1-4) (2020).

2. Regular-triangle trimer and charge order preserving the Anderson condition in the pyrochlore structure of CsW_2O_6: Y. Okamoto, H. Amano, N. Katayama, H. Sawa, K. Niki, R. Mitoka, H. Harima, T. Hasegawa, N. Ogita, Y. Tanaka, M. Takigawa, Y. Yokoyama, K. Takehana, Y. Imanaka, Y. Nakamura, H. Kishida and K. Takenaka, Nat Commun **11**, 3144-1-8 (2020).

3. *Pressure-induced phase transition in the J_1-J_2 square lattice antiferromagnet $RbMoOPO_4Cl$: H. Takeda, T. Yamauchi, M. Takigawa, H. Ishikawa and Z. Hiroi, Phys. Rev. B **103**, 104406 (2021).

4. *$PrTi_2Al_{20}$ における強四極子秩序変数の磁場によるスイッチング - 磁場に依存する四極子間相互作用について -: 谷口 貴紀 , 服部 一匡 , 橘高 俊一郎 , 瀧川 仁 , 固体物理 **55**, 245-264 (2020).

Sakakibara group

We investigated the magnetic phase transitions of the cubic chiral magnet EuPtSi by means of high-precision magnetization measurements and established the magnetic phase diagrams. The incommensurate-commensurate transition in the helical state with a tiny change in the propagation vectors was detected exclusively by the magnetization along the [111] direction. The transition temperature T_N* shifted to lower temperature with increasing H // [111]. The ground-state magnetizations of the helical state for H // [100] and [111] were examined at temperatures below 100 mK. We found evidence that the q vectors pinned to the lattice at low fields were depinned by increasing fields above 10 kOe and gradually rotated towards the field directions. Metastable skyrmion phase can be created at 60 mK by slowly cooling in a field. We obtained the ground-state magnetization of the skyrmion lattice state, showing a sharp tilted plateau structure. The transitions from the skyrmion phase to the conical phase by changing fields were perfectly discontinuous at 60 mK possibly because of the supercooled dynamics.

1. *^{105}Pd NMR and NQR study of the cubic heavy fermion system $Ce_3Pd_{20}Si_6$: I. Jakovac, M. Horvatic, E. F. Schwier, A. Prokofiev, S. Paschen, H. Mitamura, T. Sakakibara and M. S. Grbic, J. Phys.: Condens. Matter **32**, 245601(1-7) (2020).

2. *Field-Orientation Effect on Ferro-Quadrupole Order in $PrTi_2Al_{20}$: S. Kittaka, T. Taniguchi, K. Hattori, S. Nakamura, T. Sakakibara, M. Takigawa, M. Tsujimoto, A. Sakai, Y. Matsumoto and S. Nakatsuji, J. Phys. Soc. Jpn. **89**, 043701(1-4) (2020).

3. †*Heavy Fermion State of $YbNi_2Si_3$ without Local Inversion Symmetry: S. Nakamura, K. Hyodo, Y. Matsumoto, Y. Haga, H. Sato, S. Ueda, K. Mimura, K. Saiki, K. Iso, M. Yamashita, S. Kittaka, T. Sakakibara and S. Ohara, J. Phys. Soc. Jpn. **89**, 024705(1-5) (2020).

4. *Kitaev Spin Liquid Candidate Os_xCl_3 Comprised of Honeycomb Nano-Domains: K. Kataoka, D. Hirai, T. Yajima, D. Nishio-Hamane, R. Ishii, K.-Y. Choi, D. Wulferding, P. Lemmens, S. Kittaka, T. Sakakibara, H. Ishikawa, A. Matsuo, K. Kindo and Z. Hiroi, J. Phys. Soc. Jpn. **89**, 114709(1-9) (2020).

* Joint research among groups within ISSP.

5. †*Emergent spin-1 Haldane gap and ferroelectricity in a frustrated spin- 1/2 ladder: H. Ueda, S. Onoda, Y. Yamaguchi, T. Kimura, D. Yoshizawa, T. Morioka, M. Hagiwara, M. Hagihala, M. Soda, T. Masuda, T. Sakakibara, K. Tomiyasu, S. Ohira-Kawamura, K. Nakajima, R. Kajimoto, M. Nakamura, Y. Inamura, N. Reynolds, M. Frontzek, J. S. White, M. Hase and Y. Yasui, Phys. Rev. B **101**, 140408(1-6) (2020).

6. †Fully gapped superconductivity without sign reversal in the topological superconductor $PbTaSe_2$: Y. Sun, S. Kittaka, T. Sakakibara, K. Machida, R. Sankar, X. Xu, N. Zhou, X. Xing, Z. Shi, S. Pyon and T. Tamegai, Phys. Rev. B **102**, 024517(1-7) (2020).

7. †Magnetic properties of a spin-1/2 honeycomb lattice antiferromagnet: Y. Kono, T. Okabe, N. Uemoto, Y. Iwasaki, Y. Hosokoshi, S. Kittaka, T. Sakakibara and H. Yamaguchi, Phys. Rev. B **101**, 014437(1-6) (2020).

8. †Magnetic properties of a spin-2 antiferromagnet with metal-radical hybrid spins: Y. Iwasaki, T. Okabe, N. Uemoto, Y. Kono, Y. Hosokoshi, S. Nakamura, S. Kittaka, T. Sakakibara, M. Hagiwara, T. Kawakami and H. Yamaguchi, Phys. Rev. B **101**, 174412(1-6) (2020).

9. †Synthesis and Magnetic Properties of $M^{2+}Ti^{4+}$ Substituted $Ba_{12}Fe_{28}Ti_{15}O_{84}$: N. Yasuda, S. Kittaka, Y. Kono, T. Sakakibara, K. Kakizaki and K. Kamishima, J. Magn. Soc. Jpn. **44**, 2005R004(1-5) (2020).

10. *Magnetization and Thermal Expansion Properties of Quantum Spin Ice Candidate $Pr_2Zr_2O_7$: N. Tang, A. Sakai, K. Kimura, S. Nakamura, M. Fu, Y. Matsumoto, T. Sakakibara and S. Nakatsuji, JPS Conf. Proc. **30**, 011090(1-6) (2020).

11. *Single Crystal Growth and Unique Electronic States of Cubic Chiral EuPtSi and Related Compounds: Y. Ônuki, M. Kakihana, W. Iha, K. Nakaima, D. Aoki, A. Nakamura, F. Honda, M. Nakashima, Y. Amako, J. Gouchi, Y. Uwatoko, S. Nakamura, T. Sakakibara, T. Takeuchi, Y. Haga, H. Ikeda, H. Harima, M. Hedo and T. Nakama, JPS Conf. Proc. **29**, 012001(1-9) (2020).

12. *Unique Skyrmion Phases and Conduction Electrons in Cubic Chiral Antiferromagnet EuPtSi and Related Compounds: Y. Ônuki, M. Kakihana, W. Iha, K. Nakaima, D. Aoki, A. Nakamura, F. Honda, M. Nakashima, Y. Amako, J. Gouchi, Y. Uwatoko, S. Nakamura, T. Sakakibara, T. Takeuchi, Y. Haga, H. Ikeda, H. Harima, M. Hedo and T. Nakama, JPS Conf. Proc. **30**, 011008(1-11) (2020).

13. *Improved accuracy in high-frequency AC transport measurements in pulsed high magnetic fields: H. Mitamura, R. Watanuki, E. Kampert, T. Förster, A. Matsuo, T. Onimaru, N. Onozaki, Y. Amou, K. Wakiya, K. T. Matsumoto, I. Yamamoto, K. Suzuki, S. Zherlitsyn, J. Wosnitza, M. Tokunaga, K. Kindo and T. Sakakibara, Review of Scientific Instruments **91**, 125107/1-25 (2020).

14. Orientation of point nodes and nonunitary triplet pairing tuned by the easy-axis magnetization in UTe_2: S. Kittaka, Y. Shimizu, T. Sakakibara, A. Nakamura, D. Li, Y. Homma, F. Honda, D. Aoki and K. Machida, Phys. Rev. Research **2**, 032014(R)(1-6) (2020).

15. †Evidence for nematic superconductivity of topological surface states in $PbTaSe_2$: T. Le, Y. Sun, H.-K. Jin, L. Che, L. Yin, J. Li, G. Pang, C. Xu, L. Zhao, S. Kittaka, T. Sakakibara, K. Machida, R. Sankar, H. Yuan, G. Chen, X. Xu, S. Li, Y. Zhou and X. Lu, Science Bulletin **65**, 1349-1355 (2020).

16. *$PrTi_2Al_{20}$ における強四極子秩序変数の磁場によるスイッチング - 磁場に依存する四極子間相互作用について -: 谷口 貴紀 , 服部 一匡 , 橘高 俊一郎 , 瀧川 仁 , 固体物理 **55**, 245-264 (2020).

Mori group

We have successfully developed and unveiled unprecedented functional properties for the molecular materials and systems. The major achievements in 2020 are (1) to establish the molecular design strategy of anhydrous base-acid-type organic proton conductors as an electrolyte of a fuel cell for medium temperatures, (2) to investigate the alkyl-chain-length effect of the transistor properties for anthracene-based organic semiconductors, and (3) to develop the Zn complex with vapochromism induced by intermolecular electron transfer coupled with hydrogen-bond formation.

1. †Anhydrous Purely Organic Solid-State Proton Conductors: Effects of Molecular Dynamics on the Proton Conductivity of Imidazolium Hydrogen Dicarboxylates: Y. Sunairi, S. Dekura, A. Ueda, T. Ida, M. Mizuno and H. Mori, J. Phys. Soc. Jpn. **89**, 051008 (2020).

2. 水素科学の最前線、新学術領域研究「ハイドロジェノミクス」の挑戦―高速・局所移動水素と電子とのカップリングによる新発想デバイスの設計 : 森 初果 , まてりあ **60**, 165-168 (2020).

3. *A computational examination of the electric-field-induced proton transfer along the interface hydrogen bond between proton donating and accepting self-assembled monolayers: Y. Kanematsu, H. S. Kato, S. Yoshimoto, A. Ueda,

† Joint research with outside partners.

S. Yamamoto, H. Mori, J. Yoshinobu, I. Matsuda and M. Tachikawa, Chem. Phys. Lett. **741**, 137091 (2020).

4. *Vapochromism induced by intermolecular electron transfer coupled with hydrogen-bond formation in zinc dithiolene complex: T. Fujino, M. Kawamura, T. Ozaki and H. Mori, J. Mater. Chem. C **8**, 14939-14947 (2020).

5. * 水素を活かすセラミクス　プロトンー電子カップル型分子性結晶および二分子膜における機能開拓 : 森 初果 , 加藤 浩之 , 藤野 智子 , 上田 顕 , 吉信 淳 , セラミックス **56**, 88-91 (2021).

6. Effect of Alkyl Chain Length on Charge Transport Property of Anthracene-Based Organic Semiconductors: D. Zhang, S. Yokomori, R. Kameyama, C. Zhao, A. Ueda, L. Zhang, R. Kumai, Y. Murakami, H. Meng and H. Mori, ACS Appl. Mater. Interfaces **13**, 989 (2021).

7. Terahertz-field-induced polar charge order in electronic-type dielectrics: H. Yamakawa, T. Miyamoto, T. Morimoto, N. Takamura, S. Liang, H. Yoshimochi, T. Terashige, N. Kida, M. Suda, H. M. Yamamoto, H. Mori, K. Miyagawa, K. Kanoda and H. Okamoto, Nat Commun **12**, 953 (2021).

8. *The Simplest Model for Doped Poly(3,4-ethylenedioxythiophene) (PEDOT): Single-crystalline EDOT Dimer Radical Cation Salts: R. Kameyama, T. Fujino, S. Dekura, M. Kawamura, T. Ozaki and H. Mori, Chem. Eur. J. **27**, 6696 (2021).

9. Modulation of the Electronic States and Magnetic Properties of Nickel Catecholdithiolene Complex by Oxidation-coupled Deprotonation: S. Yokomori, S. Dekura, A. Ueda, R. Kumai, Y. Murakami and H. Mori, J. Mater. Chem. C (2021), accepted for publication.

Osada group

The nonlinear anomalous Hall effect (AHE) was realized in organic conductors for the first time. First, using interlayer magnetotransport, we experimentally confirmed that the weak charge ordering (CO) state of a layered organic conductor α-(BEDT-TTF)$_2$I$_3$ is a two-dimensional massive Dirac fermion (DF) state with a pair of tilted gapped Dirac cones with finite Berry curvature dipole. Next, we showed that the nonlinear AHE is measurable in the current-carrying state of this massive DF system, where the Berry curvature balance is broken between two Dirac cones due to non-equilibrium distribution. In addition, we proposed the current-field-cooling technique, which enhances the formation of single type of CO domains in experiments. Finally, we performed the transport measurement of α-(BEDT-TTF)$_2$I$_3$ in the weak CO state at 1.25GPa, and extracted nonlinear signal from current-reversed data. We successfully observed nonlinear AHE with estimated order and its rectifying characteristics.

1. Possible Current-Induced Phenomena and Domain Control in an Organic Dirac Fermion System with Weak Charge Ordering: T. Osada and A. Kiswandhi, J. Phys. Soc. Jpn. **89**, 103701/1-5 (2020).

2. Experimental Confirmation of Massive Dirac Fermions in Weak Charge-Ordering State in α-(BEDT-TTF)$_2$I$_3$: K. Yoshimura, M. Sato and T. Osada, J. Phys. Soc. Jpn. **90**, 033701/1-5 (2021).

3. Possible Nonlinear Anomalous Thermoelectric Effect in Organic Massive Dirac Fermion System: T. Osada and A. Kiswandhi, J. Phys. Soc. Jpn. **90**, 053704/1-5 (2021).

4. 黒リン超薄膜の電子構造と物性 : 長田 俊人 , 「グラフェンから広がる二次元物質の新技術と応用」, 第６章10節 , 吾郷浩樹・齋藤理一郎 , (エヌ・ティー・エス , 東京 , 2020), 437-443.

Yamashita group

We have been studying (1) quantum criticality in heavy-fermion materials by ultralow 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) developments of ultralow-temperature measurements of thermal expansion of CeCoIn$_5$ and resistivity of YbRh$_2$Si$_2$, (2) thermal-Hall measurements of Neel-type skyrmions in GaV$_4$Se$_8$, and (3) spintronic superconductor in EuSn$_2$As$_2$.

1. Thermal-transport studies of kagomé antiferromagnets: M. Yamashita, M. Akazawa, M. Shimozawa, T. Shibauchi, Y. Matsuda, H. Ishikawa, T. Yajima, Z. Hiroi, M. Oda, H. Yoshida, H.-Y. Lee, J. H. Han and N. Kawashima, J. Phys.: Condens. Matter **32**, 074001 (2020).

2. †*Heavy Fermion State of YbNi$_2$Si$_3$ without Local Inversion Symmetry: S. Nakamura, K. Hyodo, Y. Matsumoto, Y. Haga, H. Sato, S. Ueda, K. Mimura, K. Saiki, K. Iso, M. Yamashita, S. Kittaka, T. Sakakibara and S. Ohara, J. Phys. Soc. Jpn. **89**, 024705(1-5) (2020).

3. Presence and absence of itinerant gapless excitations in the quantum spin liquid candidate EtMe$_3$Sb[Pd(dmit)$_2$]$_2$: M. Yamashita, Y. Sato, T. Tominaga, Y. Kasahara, S. Kasahara, H. Cui, R. Kato, T. Shibauchi and Y. Matsuda, Phys.

* Joint research among groups within ISSP.

Rev. B **101**, 140407(R) (2020).

4. *Sample dependence of half-integer quantized thermal Hall effect in the Kitaev spin-liquid candidate α-$RuCl_3$: M. Yamashita, J. Gouchi, Y. Uwatoko, N. Kurita and H. Tanaka, Phys. Rev. B **102**, 220404(R) (2020).

5. †Ultralow temperature NMR of $CeCoIn_5$: M. Yamashita, M. Tashiro, K. Saiki, S. Yamada, M. Akazawa, M. Shimozawa, T. Taniguchi, H. Takeda, M. Takigawa and H. Shishido, Phys. Rev. B **102**, 165154 (2020).

6. ヘリウム危機の現状と今後の課題について（解説記事）：山下 穣 , 固体物理 **55**, 215-223 (2020).

7. *Thermal Hall Effects of Spins and Phonons in Kagome Antiferromagnet Cd-Kapellasite: M. Akazawa, M. Shimozawa, S. Kittaka, T. Sakakibara, R. Okuma, Z. Hiroi, H.-Y. Lee, N. Kawashima, J. H. Han and M. Yamashita, Phys. Rev. X **10**, 041059 (2020).

8. *Pressure-induced phase transition in the J_1-J_2 square lattice antiferromagnet $RbMoOPO_4Cl$: H. Takeda, T. Yamauchi, M. Takigawa, H. Ishikawa and Z. Hiroi, Phys. Rev. B **103**, 104406 (2021).

9. *Strongly correlated superconductivity in a copper-based metal-organic framework with a perfect kagome lattice: T. Takenaka, K. Ishihara, M. Roppongi, Y. Miao, Y. Mizukami, T. Makita, J. Tsurumi, S. Watanabe, J. Takeya, M. Yamashita, K. Torizuka, Y. Uwatoko, T. Sasaki, X. Huang, W. Xu, D. Zhu, N. Su, J. -G. Cheng, T. Shibauchi and K. Hashimoto, Sci. Adv. **7**, eabf3996(1-8) (2021).

Division of Condensed Matter Theory

Tsunetsugu group

We have studied several topics of strongly correlated systems and nonequilibrium phenomena. Concerning correlated systems, we have investigated the dynamics of domain wall driven by external magnetic or electric field in multiferroic materials, and found its dynamical instability to splitting. We have also reexamined phenomenological Ginzburg-Landau theory for CDW in layered compounds and found new local minima in the free-energy landscape. As for nonequilibrium phenomena, we have analyzed various aspects of high-harmonic generation in solids, including the disorder effect, dynamical point-group symmetries, and relativistic dispersion relation of Dirac semimetals. Regarding periodically-driven (Floquet) systems, we have proposed a new symmetry and derived a general expression for nonequilibrium steady states. In isolated many-body quantum systems, we have investigated conserved quantities that work as dynamical obstructions and prevent ordinary thermalization. Related to the two topics, we studied quantum quench dynamics of strongly correlated electrons in one dimension and found a clogging phenomena where particle current stops but energy current flows.

1. Generalized hydrodynamic approach to charge and energy currents in the one-dimensional Hubbard model: Y. Nozawa and H. Tsunetsugu, Phys. Rev. B **101**, 035121 (2020).

2. *Efficient Terahertz Harmonic Generation with Coherent Acceleration of Electrons in the Dirac Semimetal Cd_3As_2: B. Cheng, N. Kanda, T. N. Ikeda, T. Matsuda, P. Xia, T. Schumann, S. Stemmer, J. Itatani, N. P. Armitage and R. Matsunaga, Phys. Rev. Lett. **124**, 117402 (2020).

3. Explicit Construction of Local Conserved Quantities in the *XYZ* Spin-1/2 Chain: Y. Nozawa and K. Fukai, Phys. Rev. Lett. **125**, 090602 (2020).

4. Time Crystals Protected by Floquet Dynamical Symmetry in Hubbard Models: K. Chinzei and T. N. Ikeda, Phys. Rev. Lett. **125**, 060601 (2020).

5. Multivalley Free Energy Landscape and the Origin of Stripe and Quasi-Stripe CDW Structures in Monolayer MX_2 Compounds: K. Nakatsugawa, S. Tanda and T. N. Ikeda, Sci. Rep. **10**, 1239 (2020).

6. General description for nonequilibrium steady states in periodically driven dissipative quantum systems: T. N. Ikeda and M. Sato, Science Advances **6**, eabb4019 (2020).

7. Disorder effects on the origin of high-order harmonic generation in solids: K. Chinzei and T. N. Ikeda, Phys. Rev. Research **2**, 013033 (2020).

8. High-order nonlinear optical response of a twisted bilayer graphene: T. N. Ikeda, Phys. Rev. Research **2**, 032015(R) (2020).

9. Noncommutative generalized Gibbs ensemble in isolated integrable quantum systems: K. Fukai, Y. Nozawa, K. Kawahara and T. N. Ikeda, Phys. Rev. Research **2**, 033403 (2020).

† Joint research with outside partners.

10. Dynamics of Composite Domain Walls in Multiferroics in Magnetic Field and Their Instability: K. Kawahara and H. Tsunetsugu, J. Phys. Soc. Jpn. **90**, 014703 (2021).

11. Quadrupole Orders on the fcc Lattice: H. Tsunetsugu, T. Ishitobi and K. Hattori, J. Phys. Soc. Jpn. **90**, 043701 (2021).

12. Generalized hydrodynamics study of the one-dimensional Hubbard model: Stationary clogging and proportionality of spin, charge, and energy currents: Y. Nozawa and H. Tsunetsugu, Phys. Rev. B **103**, 035130 (2021).

Kato group

The main research subject of Kato Lab. is transport properties in mesoscopic devices. We studied (1) optimization of pumping power under adiabatic charge driving, (2) microscopic theory for spin Hall magnetoresistance, (3) Cooper-pair transport through a Josephson junction array, and (4) transport properties through a Kondo quantum dot.

1. Geometrical Optimization of Pumping Power under Adiabatic Parameter Driving: M. Hasegawa and T. Kato, J. Phys. Soc. Jpn. 89, 064706 (2020).

2. Fano-Kondo resonance versus Kondo plateau in an Aharonov-Bohm ring with an embedded quantum dot: M. Eto and R. Sakano, Phys. Rev. B **102**, 245402 (2020).

3. Field-induced SU(4) to SU(2) Kondo crossover in a half-filling nanotube dot: Spectral and finite-temperature properties: Y. Teratani, R. Sakano, T. Hata, T. Arakawa, M. Ferrier, K. Kobayashi and A. Oguri, Phys. Rev. B **102**, 165106 (2020).

4. Microscopic theory of spin Hall magnetoresistance: T. Kato, Y. Ohnuma and M. Matsuo, Phys. Rev. B **102**, 094437 (2020).

5. Fermi Liquid Theory for Nonlinear Transport through a Multilevel Anderson Impurity: Y. Teratani, R. Sakano and A. Oguri, Phys. Rev. Lett. **125**, 216801 (2020).

6. Cooper-Pair Tunneling in Small Josephson Junction Arrays Under Radio-Frequency Irradiation: G. M. Kanyolo, K. Takeda, Y. Mizugaki, T. Kato and H. Shimada, J. Low Temp. Phys. **201**, 269 (2020).

7. Effects of Tunnel-coupling Asymmetries on Fermi-liquid Transport through an Anderson Impurity: K. Tsutsumi, Y. Teratani, A. Oguri and R. Sakano, JPS conf. ser. **30**, 011174(1-6) (2020).

8. †*DSQSS: Discrete Space Quantum Systems Solver: Y. Motoyama, K. Yoshimi, A. Masaki-Kato, T. Kato and N. Kawashima, Computer Physics Communications **264**, 107944 (2021).

9. 非平衡状態にある近藤効果（その 2）近藤効果入門 1: 阪野 塁 , 小栗 章 , 固体物理 **55**, 47-54 (2020).

Division of Nanoscale Science

Katsumoto group

We further advanced the study of flying qubits using spin-polarized quantum Hall edge states. In particular, we improved the beam splitter that splits the electron beam into two channels, and increased the splitting probability from a few percent to 50%, and obtained a beam splitter equivalent to a half mirror in quantum optics. The interferometer using this showed high visibility of over 70%. In the super-normal-super (SNS) junction, the decrease of the superconducting critical current with the positive gate voltage has been unexplained. We have found the phenomenon can be interpreted as the decrease of quantum coherence in the Andreev bound state by the in-plane voltage.

1. Gate-controlled unitary operation on flying spin qubits in quantum Hall edge states: T. Shimizu, T. Nakamura, Y. Hashimoto, A. Endo and S. Katsumoto, Phys. Rev. B **102**, 235302 (2020).

2. †Optoelectronic properties of laser-beam-patterned few-layer lateral MoS_2 Schottky junctions: Y. Nagamine, J. Sato, Y. Qian, T. Inoue, T. Nakamura, S. Maruyama, S. Katsumoto and J. Haruyama, Appl. Phys. Lett. **117**, 043101 (2020).

3. *Extracting the Chiral Contribution to the Negative Longitudinal Magnetoresistance in Epitaxial $Pr_2Ir_2O_7$ Thin Films: T. Ohtsuki, Z. Tian, A. Endo, M. Halim, S. Katsumoto, Y. Kohama, K. Kindo, M. Lippmaa and S. Nakatsuji, JPS Conf. Proc. **30**, 011181 (1-6) (2020).

4. †Room-temperature quantum spin Hall phase in laser-patterned few-layer 1T'- MoS_2: N. Katsuragawa, M. Nishizawa, T. Nakamura, T. Inoue, S. Pakdel, S. Maruyama, S. Katsumoto, J. J. Palacios and J. Haruyama, Commun Mater **1**, 51

---

* Joint research among groups within ISSP.

(2020).

5. 薄膜材料の電気特性： 勝本　信吾，「2020 年版薄膜作製応用ハンドブック」，第２章，權田俊一，(NTS 出版，東京，2020), 39-79.

Otani group

This year, we have studied the following topics: spin conversion behaviors in bulk, the interfaces and the surfaces, the magnon-phonon or magnon-magnon coupling in ferromagnetic heterostructures, and antiferromagnetic spintronics. I summarize the remarkable achievements this year below. We have established a phenomenological model explaining the contributions of bulk and interfacial spin relaxation. Our study of transverse magnetoresistance in magnetic heterostructure evidenced the spin swapping at the Rashba interface. We have experimentally demonstrated the conversion of acoustically induced spin currents to the charge current using a metal/oxide Rashba interface. This study has also shown significant enhancement of magnon-phonon coupling using the Brag reflector cavity structure. Besides, our international collaboration showed a large nonlinear ferromagnetic resonance shift due to strong magnon-magnon coupling. We had another collaborative project on skyrmion strings that clarified their detailed propagation dynamics. This year, there are two exciting breakthroughs; Electrical manipulation of a topological antiferromagnetic state and Emergent electromagnetic induction in a helical-spin magnet, both of which appeared in Nature magazine.

1. Underlayer material dependent symmetric and asymmetric behavior of voltage-controlled magnetic anisotropy in CoFeB films: B. Rana, K. Miura, H. Takahashi and Y. Otani, J. Phys.: Condens. Matter **32**, 414002 (2020).

2. Electric-field control of interfacial in-plane magnetic anisotropy in CoFeB/MgO junctions: A. Deka, B. Rana, R. Anami, K. Miura, H. Takahashi, Y. Otani and Y. Fukuma, Phys. Rev. B **101**, 174405 (2020).

3. Large nonlinear ferromagnetic resonance shift and strong magnon-magnon coupling in $Ni_{80}Fe_{20}$ nanocross array: K. Adhikari, S. Sahoo, A. K. Mondal, Y. Otani and A. Barman, Phys. Rev. B **101**, 054406 (2020).

4. Phenomenological model for the direct and inverse Edelstein effects: H. Isshiki, P. Muduli, J. Kim, K. Kondou and Y. Otani, Phys. Rev. B **102**, 184411 (2020).

5. *Effect of sample size on anomalous Nernst effect in chiral antiferromagnetic Mn_3Sn devices: H. Narita, T. Higo, M. Ikhlas, S. Nakatsuji and Y. Otani, Appl. Phys. Lett. **116**, 072404 (2020).

6. Enhancement of acoustic spin pumping by acoustic distributed Bragg reflector cavity: Y. Hwang, J. Puebla, M. Xu, A. Lagarrigue, K. Kondou and Y. Otani, Appl. Phys. Lett. **116**, 252404 (2020).

7. Evidence for spin swapping from modulation of transverse resistance in magnetic heterostructures with Rashba interface: H. Kim, S. Karube, J. Borge, J. Kim, K. Kondou and Y. Otani, Appl. Phys. Lett. **116**, 122403 (2020).

8. *Magneto-optical Kerr effect in a non-collinear antiferromagnet Mn_3Ge: M. Wu, H. Isshiki, T. Chen, T. Higo, S. Nakatsuji and Y. Otani, Appl. Phys. Lett. **116**, 132408 (2020).

9. *Electrical manipulation of a topological antiferromagnetic state: H. Tsai, T. Higo, K. Kondou, T. Nomoto, A. Sakai, A. Kobayashi, T. Nakano, K. Yakushiji, R. Arita, S. Miwa, Y. Otani and S. Nakatsuji, Nature **580**, 608-613 (2020).

10. Emergent electromagnetic induction in a helical-spin magnet: T. Yokouchi, F. Kagawa, M. Hirschberger, Y. Otani, N. Nagaosa and Y. Tokura, Nature **586**, 232 (2020).

11. *Chirality-induced effective magnetic field in a phthalocyanine molecule: S. Miwa, K. Kondou, S. Sakamoto, A. Nihonyanagi, F. Araoka, Y. Otani and D. Miyajima, Appl. Phys. Express **13**, 113001 (1-4) (Spotlights 2020) (2020).

12. Acoustic ferromagnetic resonance and spin pumping induced by surface acoustic waves: J. Puebla, M. Xu, B. Rana, K. Yamamoto, S. Maekawa and Y. Otani, J. Phys. D: Appl. Phys. **53**, 264002 (2020).

13. *Structural and magnetic properties of Mn_3Ge films with Pt and Ru seed layers: A. Kobayashi, T. Higo, S. Nakatsuji and Y. Otani, AIP Advances **10**, 015225(1-6) (2020).

14. Nonlinear Control of Damping Constant by Electric Field in Ultrathin Ferromagnetic Films: B. Rana, C. A. Akosa, K. Miura, H. Takahashi, G. Tatara and Y. Otani, Phys. Rev. Applied **14**, 014037 (2020).

15. Nonreciprocal surface acoustic wave propagation via magneto-rotation coupling: M. Xu, K. Yamamoto, J. Puebla, K. Baumgaertl, B. Rana, K. Miura, H. Takahashi, D. Grundler, S. Maekawa and Y. Otani, Sci. Adv. **6**, eabb1724 (2020).

16. Voltage controlled on-demand magnonic nanochannels: S. Choudhury, A. K. Chaurasiya, A. K. Mondal, B. Rana, K. Miura, H. Takahashi, Y. Otani and A. Barman, Sci. Adv. **6**, eaba5457 (2020).

† Joint research with outside partners.

17. Phase boundary exchange coupling in the mixed magnetic phase regime of a Pd-doped FeRh epilayer: J. R. Massey, K. Matsumoto, M. Strungaru, R. C. Temple, T. Higo, K. Kondou, R. F. L. Evans, G. Burnell, R. W. Chantrell, Y. Otani and C. H. Marrows, Phys. Rev. Materials **4**, 024403(1-11) (2020).

18. Propagation dynamics of spin excitations along skyrmion strings: S. Seki, M. Garst, J. Waizner, R. Takagi, N. D. Khanh, Y. Okamura, K. Kondou, F. Kagawa, Y. Otani and Y. Tokura, Nat Commun **11**, 256 (2020).

19. *Electrical nucleation, displacement, and detection of antiferromagnetic domain walls in the chiral antiferromagnet Mn_3Sn: S. Sugimoto, Y. Nakatani, Y. Yamane, M. Ikhlas, K. Kondou, M. Kimata, T. Tomita, S. Nakatsuji and Y. Otani, Commun Phys **3**, 111 (2020).

20. Creation of magnetic skyrmions by surface acoustic waves: T. Yokouchi, S. Sugimoto, B. Rana, S. Seki, N. Ogawa, S. Kasai and Y. Otani, Nat. Nanotechnol. **15**, 361 (2020).

21. Spintronic devices for energy-efficient data storage and energy harvesting: J. Puebla, J. Kim, K. Kondou and Y. Otani, Commun Mater **1**, 24 (2020).

22. Nontrivial torque generation by orbital angular momentum injection in ferromagnetic-metal/Cu/Al_2O_3 trilayers: J. Kim, D. Go, H. Tsai, D. Jo, K. Kondou, H.-W. Lee and Y. Otani, Phys. Rev. B **103**, L020407 (2021).

23. *Domain structure and domain wall dynamics in topological chiral antiferromagnets from the viewpoint of magnetic octupole: Y. Otani and T. Higo, Appl. Phys. Lett. **118**, 040501 (2021).

24. *Omnidirectional Control of Large Electrical Output in a Topological Antiferromagnet: T. Higo, Y. Li, K. Kondou, D. Qu, M. Ikhlas, R. Uesugi, D. Nishio-Hamane, C. L. Chien, Y. Otani and S. Nakatsuji, Adv. Funct. Mater. **31**, 2008971-12 (2021).

25. *Spin-orbit torque switching of the antiferromagnetic state in polycrystalline Mn_3Sn/Cu/heavy metal heterostructures: H. Tsai, T. Higo, K. Kondou, A. Kobayashi, T. Nakano, K. Yakushiji, S. Miwa, Y. Otani and S. Nakatsuji, AIP Advances **11**, 045110 (1-6) (2021).

26. Strain-induced Megahertz Oscillation and Stable Velocity of an Antiferromagnetic Domain Wall: F. Chen, X. Ge, W. Luo, R. Xing, S. Liang, X. Yang, L. You, R. Xiong, Y. Otani and Y. Zhang, Phys. Rev. Applied **15**, 014030 (2021).

27. *Fabrication of polycrystalline Weyl antiferromagnetic Mn_3Sn thin films on various seed layers: T. Nakano, T. Higo, A. Kobayashi, S. Miwa, S. Nakatsuji and K. Yakushiji, Phys. Rev. Materials **5**, 054402 (1-9) (2021).

28. Nanochannels for spin-wave manipulation in $Ni_{80}Fe_{20}$ nanodot arrays: S. Sahoo, S. N. Panda, S. Barman, Y. Otani and A. Barman, Journal of Magnetism and Magnetic Materials **522**, 167550 (2021).

29. *Giant Effective Damping of Octupole Oscillation in an Antiferromagnetic Weyl Semimetal: S. Miwa, S. Iihama, T. Nomoto, T. Tomita, T. Higo, M. Ikhlas, S. Sakamoto, Y. Otani, S. Mizukami, R. Arita and S. Nakatsuji, Small Science **1**, 2000062 (1-8) (2021).

30. *Large Hall Signal due to Electrical Switching of an Antiferromagnetic Weyl Semimetal State: H. Tsai, T. Higo, K. Kondou, S. Sakamoto, A. Kobayashi, T. Matsuo, S. Miwa, Y. Otani and S. Nakatsuji, Small Science **1**, 2000025 (1-9) (2021).

Komori group

Distribution of local lattice distortion due to the hetero atomic overlayer is investigated using scanning tunneling microscopy(STM) on the Cu(111) surface covered by hexagonal Fe_2N atomic layer. We utilize the moiré pattern to reach a higher spatial resolution than simple STM observations. The distortion can be greatly affected by the formation of atomic impurities at the subsurface. Ultrathin films of $L1_0$-type FeNi are grown using nitrogen-surfactant epitaxy on the Cu(001) substrate. Well-ordered films with little intermixing among Cu, Fe and Ni atoms are realized by optimizing the substrate temperature during the Fe and Ni deposition and the post-annealing temperature. Their ferromagnetic properties are studied by soft X-ray magnetic circular dichroism. An out-of-plane magnetocrystalline anisotropy is large enough for dominating the film shape anisotropy. Electronic structure of 3~4-degree twisted bilayer graphene is investigated using angle-resolved photoemission spectroscopy with synchrotron light. The interface between the two graphene sheets of the present samples is made in a high vacuum. Owing to the strong interlayer interaction, significant band modifications including replica bands are observed at the energy near the Dirac point and crossing points of the Dirac bands. In particular, partial flat bands appear with changes in the Dirac velocity, depending on the twist angles. The observed band structure is consistent with the result of tight-binding calculations.

1. †**Orbital Angular Momentum Induced Spin Polarization of 2D Metallic Bands: T. Kobayashi, Y. Nakata, K. Yaji, T. Shishidou, D. Agterberg, S. Yoshizawa, F. Komori, S. Shin, M. Weinert, T. Uchihashi and K. Sakamoto, Phys. Rev.

---

* Joint research among groups within ISSP.

Lett. **125**, 176401, 1-6 (2020).

2. Sensing surface lattice strain with Kondo resonance of single Co adatom: K. Iwata, T. Miyamachi, E. Minamitani and F. Komori, Appl. Phys. Lett. **116**, 051604, 1-4 (2020).

3. †Twisted bilayer graphene fabricated by direct bonding in a high vacuum: H. Imamura, A. Visikovskiy, R. Uotani, T. Kajiwara, H. Ando, T. Iimori, K. Iwata, T. Miyamachi, K. Nakatsuji, K. Mase, T. Shirasawa, F. Komori and S. Tanaka, Appl. Phys. Express **13**, 075004, 1-5 (2020).

4. *Edge-state correlation accelerates metal-insulator transition in topological semimetal nanofilms: S. Ito, M. Arita, J. Haruyama, B. Feng, W. -C. Chen, H. Namatame, M. Taniguchi, C. -M. Cheng, G. Bian, S. -J. Tang, T. -C. Chiang, O. Sugino, F. Komori and I. Matsuda, Science Advances **6**, eaaz5015 (7 pages) (2020).

5. †*Topological Surface State of Bi_2Se_3 Modified by Adsorption of Organic Donor Molecule Tetrathianaphthacene: T. Kitazawa, K. Yaji, K. Shimozawa, H. Kondo, T. Yamanaka, H. Yaguchi, Y. Ishida, K. Kuroda, A. Harasawa, T. Iwahashi, Y. Ouchi, F. Komori, S. Shin and K. Kanai, Adv. Mater. Interfaces **7**, 2000524, 1-8 (2020).

6. Realizing large out-of-plane magnetic anisotropy in $L1_0$ FeNi films grown by nitrogen-surfactant epitaxy on Cu(001): K. Kawaguchi, T. Miyamachi, T. Iimori, Y. Takahashi, T. Hattori, T. Yokoyama, M. Kotsugi and F. Komori, Phys. Rev. Materials **4**, 054403, 1-7 (2020).

7. *Fully spin-polarized bulk states in ferroelectric GeTe: J. Krempaský, M. Fanciulli, L. Nicolaï, J. Minár, H. Volfová, O. Caha, V. V. Volobuev, J. Sánchez-Barriga, M. Gmitra, K. Yaji, K. Kuroda, S. Shin, F. Komori, G. Springholz and J. Hugo Dil, Phys. Rev. Research **2**, 013107,1-7 (2020).

8. Hexagonal iron nitride monolayer on Cu(001): Zigzag-line-in-trough alignment: M. Yamada, K. Ienaga, Y. Takahashi, T. Miyamachi and F. Komori, Surface Science **700**, 121679, 1-9 (2020).

9. Subatomic Distortion of Surface Monolayer Lattice Visualized by Moiré Pattern: T. Hattori, N. Kawamura, T. Iimori, T. Miyamachi and F. Komori, Nano Lett. **21**, 2406-2411 (2021).

10. †*Atomic-layer Rashba-type superconductor protected by dynamic spin-momentum locking: S. Yoshizawa, T. Kobayashi, Y. Nakata, K. Yaji, K. Yokota, F. Komori, S. Shin, K. Sakamoto and T. Uchihashi, Nat Commun **12**, 1462 (2021).

11. †Electronic structure of 3 degree-twisted bilayer graphene on 4H-SiC(0001): T. Iimori, A. Visikovskiy, H. Imamura, T. Miyamachi, M. Kitamura, K. Horiba, H. Kumigashira, K. Mase, K. Nakatsuji, S. Tanaka and F. Komori, Phys. Rev. Material **5** (2021), in print.

Hasegawa group

We have investigated monolayer superconducting materials using low temperature scanning tunneling microscopy (STM). In the case of two-dimensional superconductors, it has been known that the superconductivity is directly transformed into insulator by introducing defects or applying magnetic field. Recent transport measurements on superconducting crystalline thin films, however, revealed the presence of metallic phases during the super-insulator transitions. In order to elucidate the phenomena we performed local superconducting gap measurements by STM on atomically-thin well-ordered Pb superconductors under the perpendicular magnetic field. We observed the metallic phase and found by using vicinal substrates to introduce regularly-arranged steps as scatterers that the critical temperature is reduced but the superconducting gap remains the same. Analyzing these peculiar microscopic features will provide a new scenario on the super-insulator transition. We are now developing a new local method to probe spin dynamics of nano-size structures including single atoms/molecules by detecting electron/ferro-magnetic resonances based on spin-polarized STM. We have introduced radio-frequency (RF) cables into the STM head and successfully detected response of the RF irradiation in spin-polarized tunneling current. Using spin-polarized STM we have characterized magnetic properties of FeCo alloy island structures and found that the magnetoanisotropy can be significantly reduced by the alloying. We plan to use the alloyed islands as a sample for the resonance detection.

1. Numerical calculation of the potential distribution on the Si(111)-7 × 7 surface for scanning tunneling potentiometry: M. Hamada, H.-H. Yang and Y. Hasegawa, Jpn. J. Appl. Phys. **59**, SN1016 1-6 (2020).

2. Si(111)-7×7 表面上の一次元欠陥における電気伝導評価 : 浜田 雅之 , 長谷川 幸雄 , 表面と真空 **63**, 431-436 (2020).

3. Enhanced critical magnetic field for monoatomic-layer superconductor by Josephson junction steps: F. Oguro, Y. Sato, K. Asakawa, M. Haze and Y. Hasegawa, Phys. Rev. B **103**, 085416 1-7 (2021).

† Joint research with outside partners.

Lippmaa group

We concluded the project on fabricating iridate pyrochlore thin films by solid-state epitaxy. The behavior of iridium and other noble metals in the oxide thin film growth process was studied. In particular, the spontaneous phase separation of noble metals was studied in perovskite and pyrochlore lattices. Several techniques were studied for controlling the sheet carrier density in oxide heterostructures with delta-doping layers. The $SrTiO_3$ / $LaTiO_3$ system was used in these experiments. A new sacrificial buffer layer process was developed for fabricating strain-free free-standing oxide thin films.

1. *Growth of $Pr_2Ir_2O_7$ thin films using solid phase epitaxy: T. Ohtsuki, Z. Tian, M. Halim, S. Nakatsuji and M. Lippmaa, J. Appl. Phys. **127**, 035303 (1-9) (2020).
2. Noble metal clustering and nanopillar formation in an oxide matrix: M. Lippmaa, S. Kawasaki, R. Takahashi and T. Yamamoto, Jpn. J. Appl. Phys. **59**, 010501 (1-9) (2020).
3. Tuning the carrier density in $SrTiO_3/LaTiO_3/SrTiO_3$ quantum wells: J. N. Lee, X. Hou, R. Takahashi and M. Lippmaa, Appl. Phys. Lett. **116**, 171601 (1-5) (2020).
4. † 水溶性犠牲層を用いた単結晶薄膜分離技術 : 高橋 竜太 , リップ マーミック , セラミックデータブック **48**, 71-75 (2020).
5. *Extracting the Chiral Contribution to the Negative Longitudinal Magnetoresistance in Epitaxial $Pr_2Ir_2O_7$ Thin Films: T. Ohtsuki, Z. Tian, A. Endo, M. Halim, S. Katsumoto, Y. Kohama, K. Kindo, M. Lippmaa and S. Nakatsuji, JPS Conf. Proc. **30**, 011181 (1-6) (2020).
6. Sacrificial Water-Soluble BaO Layer for Fabricating Free-Standing Piezoelectric Membranes: R. Takahashi and M. Lippmaa, ACS Appl. Mater. Interfaces **12**, 25042-25049 (2020).
7. Nanopillar composite electrodes for solar-driven water splitting: M. Lippmaa, S. Kawasaki, R. Takahashi and T. Yamamoto, MRS Bulletin **46**, 142-151 (2021).
8. *Observation and control of the weak topological insulator state in $ZrTe_5$: P. Zhang, R. Noguchi, K. Kuroda, C. Lin, K. Kawaguchi, K. Yaji, A. Harasawa, M. Lippmaa, S. Nie, H. Weng, V. Kandyba, A. Giampietri, A. Barinov, Q. Li, G. D. Gu, S. Shin and T. Kondo, Nat. Commun. **12**, 406 (2021).
9. †Realization of closed-loop optimization of epitaxial titanium nitride thin-film growth via machine learning: I. Ohkubo, Z. Hou, J. N. Lee, T. Aizawa, M. Lippmaa, T. Chikyow, K. Tsuda and T. Mori, Mater. Today Phys. **16**, 100296 (1-6) (2021).

Functional Materials Group

Yoshinobu group

We conducted several research projects in the fiscal year 2020: (1) The surface chemistry of hydrogen and formic acid on Cu step surfaces and Pd-Cu single atom alloy model catalysts studied by SR-PES, IRAS, HREELS and TPD. (2) The adsorption and desorption of CO_2 on Pt(997) studied by TPD and SR-XPS. (3) The adsorption and desorption of CH_4 on Pt(997) studied by IRAS, TPD and SR-XPS. (4) In-situ SR-XPS study of CVD graphene on a Cu surface. (5) AP-XPS study of Pd deposited MoS_2 under hydrogen pressure. (6) THz field induced second harmonic light modulation on Pt(111).

1. *Emergence of nearly flat bands through a kagome lattice embedded in an epitaxial two-dimensional Ge layer with a bitriangular structure: A. Fleurence, C. -C. Lee, R. Friedlein, Y. Fukaya, S. Yoshimoto, K. Mukai, H. Yamane, N. Kosugi, J. Yoshinobu, T. Ozaki and Y. Yamada-Takamura, Phys. Rev. B **102**, 201102 (2020).
2. *Formation of BN-covered silicene on ZrB_2/Si(111) by adsorption of NO and thermal processes: J. Yoshinobu, K. Mukai, H. Ueda, S. Yoshimoto, S. Shimizu, T. Koitaya, H. Noritake, C.-C. Lee, T. Ozaki, A. Fleurence, R. Friedlein and Y. Yamada-Takamura, J. Chem. Phys. **153**, 064702 (2020).
3. The roles of step-site and zinc in surface chemistry of formic acid on clean and Zn-modified Cu(111) and Cu(997) surfaces studied by HR-XPS, TPD, and IRAS: Y. Shiozawa, T. Koitaya, K. Mukai, S. Yoshimoto and J. Yoshinobu, J. Chem. Phys. **152**, 044703 (2020).
4. *A computational examination of the electric-field-induced proton transfer along the interface hydrogen bond between proton donating and accepting self-assembled monolayers: Y. Kanematsu, H. S. Kato, S. Yoshimoto, A. Ueda, S. Yamamoto, H. Mori, J. Yoshinobu, I. Matsuda and M. Tachikawa, Chem. Phys. Lett. **741**, 137091 (2020).
5. †*Atomistic-Level Description of GaN/Water Interface by a Combined Spectroscopic and First-Principles Computa-

* Joint research among groups within ISSP.

tional Approach: M. Sato, Y. Imazeki, T. Takeda, M. Kobayashi, S. Yamamoto, I. Matsuda, J. Yoshinobu, Y. Nakano and M. Sugiyama, J. Phys. Chem. C **124**, 12466 (2020).

6. C–H Bond Activation of Methane through Electronic Interaction with Pd(110): T. Koitaya, A. Ishikawa, S. Yoshimoto and J. Yoshinobu, J. Phys. Chem. C **125**, 1368 (2021).

7. * 水素を活かすセラミクス　プロトンー電子カップル型分子性結晶および二分子膜における機能開拓：森 初果 , 加藤 浩之 , 藤野 智子 , 上田 顕 , 吉信 淳 , セラミックス **56**, 88-91 (2021).

8. Role of Intermolecular Interactions in the Catalytic Reaction of Formic Acid on Cu(111): A. Shiotari, S. E. M. Putra, Y. Shiozawa, Y. Hamamoto, K. Inagaki, Y. Morikawa, Y. Sugimoto, J. Yoshinobu and I. Hamada, Small **2021**, 2008010 (2021).

9. †*Structure and electronic structure of van der Waals interfaces at a Au(111) surface covered with a well-ordered molecular layer of n-alkanes: H. Mizushima, H. Koike, K. Kuroda, K. Yaji, A. Harasawa, Y. Ishida, M. Nakayama, K. Mase, K. Mukai, T. Kitazawa, T. Kondo, J. Yoshinobu, S. Shin and K. Kanai, Applied Surface Science **535**, 147673 (2021).

10. 2020年版薄膜作製応用ハンドブック（權田俊一監修）第３編第２章第７節「薄膜の表面・界面制御と信頼性」(p.883-p.888): 吉信 淳 , (NTS, Tokyo, Japan, 2020).

Akiyama group

In 2020, which is the last year of our NEDO laser project started in 2018, we made development (fab-less production) and characterizations of gain-sitched 1030-1060 nm InGaAs laser diodes (LDs) for short seed-pulse generation below 10 ps, and indeed demonstrated 8 ps pulses generated directly from our developed LDs. We also studied multi-section LDs with strong nonlinearity for short-pulse generation mechanism analysis. Our study in 2020 on novel solar cells included lead-halide Perovskite solar cells, space-use multi-junction solar cells, and textured solar cells. Our study on bio- and chemical-physics has been extended to new luciferin analogs and caged-luciferins.

1. Accurate modeling of electron-hole binding in CuCl. I. Exciton states: S. V. Nair, J. Usukura and E. Tokunaga, Phys. Rev. B **102**, 075202 (2020).

2. Accurate modeling of electron-hole binding in CuCl. II. Biexciton wavefunction: J. Usukura, S. V. Nair and E. Tokunaga, Phys. Rev. B **102**, 075203 (2020).

3. *In situ* wavelength tuning of quantum-dot single-photon sources integrated on a CMOS-processed silicon waveguide: R. Katsumi, Y. Ota, A. Osada, T. Tajiri, T. Yamaguchi, M. Kakuda, S. Iwamoto, H. Akiyama and Y. Arakawa, Appl. Phys. Lett. **116**, 041103 (2020).

4. *Quantum-mechanical hydration plays critical role in the stability of firefly oxyluciferin isomers: State-of-the-art calculations of the excited states: Y. Noguchi, M. Hiyama, M. Shiga, H. Akiyama and O. Sugino, J. Chem. Phys. **153**, 201103 (2020).

5. Exciton Localization and Enhancement of the Exciton–LO Phonon Interaction in a $CsPbBr_3$ Single Crystal: K. Shibata, J. Yan, Y. Hazama, S. Chen and H. Akiyama, J. Phys. Chem. C **124**, 18257 (2020).

6. Theoretical Study of the Wavelength Selection for the Photocleavage of Coumarin-caged D-luciferin: J. Usukura, M. Hiyama, M. Kurata, Y. Hazama, X. Qiu, F. M. Winnik, H. Akiyama and N. Koga, Photochem Photobiol **96**, 805-814 (2020).

7. Quantitative immunohistochemistry using an antibody-fused bioluminescent protein: K.-Y. Wang, C. Wu, S. Shimajiri, H. Kubota, H. Akiyama and Y. Ohmiya, BioTechnique **64**, 302-306 (2020).

8. High performance single-mode vertical cavity surface emitting lasers based on $CsPbBr_3$ nanocrystals with simplified processing: C. Zhao, J. Tao, J. Tian, G. Weng, H. Liu, Y. Liu, J. Yan, S. Chen, Y. Pan, X. Hu, S. Chen, H. Akiyama and J. Chu, Chemical Engineering Journal **(online)**, 127660 (2020).

9. Lasing operation in the $CsPbBr_3$ perovskite micron hemisphere cavity grown by chemical vapor deposition: H. Zhang, C. Zhao, S. Chen, J. Tian, J. Yan, G. Weng, X. Hu, J. Tao, Y. Pan, S. Chen, H. Akiyama and J. Chu, Chemical Engineering Journal **389**, 124395 (2020).

10. Absolute electroluminescence imaging with distributed circuit modeling: Excellent for solar-cell defect diagnosis: J. Hong, Y. Wang, Y. Chen, X. Hu, G. Weng, S. Chen, H. Akiyama, Y. Zhang, B. Zhang and J. Chu, Prog Photovolt Res Appl **28**, 295 (2020).

† Joint research with outside partners.

11. Modeling and design for low-cost multijunction solar cell via light-trapping rear texture technique: Applied in InGaP/GaAs/InGaAs triple junction: L. Zhu, Y. Hazama, A. Reddy, K. Watanabe, Y. Nakano, M. Sugiyama and H. Akiyama, Prog Photovolt Res Appl **28**, 251 (2020).

12. Practical target values of Shockley–Read–Hall recombination rates in state-of-the-art triple-junction solar cells for realizing conversion efficiencies within 1% of the internal radiative limit: T. Nakamura, M. Imaizumi, H. Akiyama and Y. Okada, Prog Photovolt Res Appl **28**, 417 (2020).

13. Quantitative study of electron tunneling dynamics in asymmetric coupled InGaN/GaN quantum wells: G. Weng, Y. Liu, S. Chen, T. Ito, X. Hu, C. Zhao, J. Liu, J. Chu and H. Akiyama, Applied Optics **59**, 6231-6236 (2020).

14. Importance of Interfacial Passivation in the High Efficiency of Sb_2Se_3 Thin-Film Solar Cells: Numerical Evidence: Y. Chen, Y. Wang, R. Wang, X. Hu, J. Tao, G.-E. Weng, C. Zhao, S. Chen, Z. Zhu, J. Chu and H. Akiyama, ACS Appl. Energy Mater. **11**, 10415–10422 (2020).

15. [*]Direct generation of sub-picosecond pulse via multi-section gain switching: T. Nakamura, T. Ito, H. Nakamae, C. Kim, Y. Hazama, Y. Kobayashi, R. Kuroda and H. Akiyama, Opt. Lett. **46**, 1277 (2021).

16. Fabricating over 7%-efficient $Sb_2(S,Se)_3$ thin-film solar cells by vapor transport deposition using Sb_2Se_3 and Sb_2S_3 mixed powders as the evaporation source: X. Hu, J. Tao, R. Wang, Y. Wang, Y. Pan, G. Weng, X. Luo, S. Chen, Z. Zhu, J. Chu and H. Akiyama, Journal of Power Sources **493**, 229737 (2021).

17. Superior single-mode lasing in a self-assembly $CsPbX_3$ microcavity over an ultrawide pumping wavelength range: G. Weng, J. Yan, S. Chen, C. Zhao, H. Zhang, J. Tian, Y. Liu, X. Hu, J. Tao, S. Chen, Z. Zhu, H. Akiyama and J. Chu, Photon. Res. **9**, 54 (2021).

18. Electron–Hole Plasma Lasing Dynamics in $CsPbCl_mBr_{3-m}$ Microplate Lasers: G. Weng, J. Tian, S. Chen, J. Yan, H. Zhang, Y. Liu, C. Zhao, X. Hu, X. Luo, J. Tao, S. Chen, Z. Zhu, J. Chu and H. Akiyama, ACS Photonics **8**, 787 (2021).

19. Adaptive automatic solar cell defect detection and classification based on absolute electroluminescence imaging: Y. Wang, L. Li, Y. Sun, J. Xu, Y. Jia, J. Hong, X. Hu, G. Weng, X. Luo, S. Chen, Z. Zhu, J. Chu and H. Akiyama, Energy **229**, 120606 (2021).

20. Enhanced Magneto-Optical Kerr Effect of GaAs-Based P-N Junctions in the Terahertz Range: K. Miyagawa, M. Nagai, M. Ashida, C. Kim and H. Akiyama, J Infrared Milli Terahz Waves **42**, 325 (2021).

Sugino group

We have studied the density functional theory for molecules and condensed matters either in the ground state or in the excited states. We have also studies energy-materials such as lithium-ion battery, solid-state battery and fuel-cell and bio-materials such as oxyluciferin of firefly. We have also contributed to get theoretical interpretation of experiments. All are based on the first-principles calculations.

1. Hydrogen at Electrochemical Interfaces: O. Sugino, J. Phys. Soc. Jpn. **89**, 051013 (2020).

2. [†]Nuclear quantum effect for hydrogen adsorption on Pt(111): L. Yan, Y. Yamamoto, M. Shiga and O. Sugino, Phys. Rev. B **101**, 165414 (2020).

3. [*]Quantum-mechanical hydration plays critical role in the stability of firefly oxyluciferin isomers: State-of-the-art calculations of the excited states: Y. Noguchi, M. Hiyama, M. Shiga, H. Akiyama and O. Sugino, J. Chem. Phys. **153**, 201103 (2020).

4. [†]Machine learning exchange-correlation potential in time-dependent density-functional theory: Y. Suzuki, R. Nagai and J. Haruyama, Phys. Rev. A **101**, 050501 (2020).

5. [†]Structural Variation in Carbonate Electrolytes by the Addition of Li Salts Studied by X-Ray Total Scattering: K. Kimura, K. Hayashi, H. Kiuchi, M. Morita, J. Haruyama, M. Otani, H. Sakaebe, F. Fujisaki, K. Mori, M. Yonemura, Y. Takabayashi, T. Nakatani, S. Fujinami, T. Fukunaga and E. Matsubara, Phys. Status Solidi B **257**, 2000100 (2020).

6. [†]Dopant arrangements in Y-doped $BaZrO_3$ under processing conditions and their impact on proton conduction: a large-scale first-principles thermodynamics study: S. Kasamatsu, O. Sugino, T. Ogawa and A. Kuwabara, J. Mater. Chem. A **8**, 12674 (2020).

7. [*]Edge-state correlation accelerates metal-insulator transition in topological semimetal nanofilms: S. Ito, M. Arita, J. Haruyama, B. Feng, W. -C. Chen, H. Namatame, M. Taniguchi, C. -M. Cheng, G. Bian, S. -J. Tang, T. -C. Chiang,

[*] Joint research among groups within ISSP.

O. Sugino, F. Komori and I. Matsuda, Science Advances **6**, eaaz5015 (7 pages) (2020).

8. [†]Surface-state Coulomb repulsion accelerates a metal-insulator transition in topological semimetal nanofilms: S. Ito, M. Arita, J. Haruyama, B. Feng, W. -C. Chen, H. Namatame, M. Taniguchi, C. -M. Cheng, G. Bian, S. -J. Tang, T. -C. Chiang, O. Sugino, F. Komori and I. Matsuda, Sci. Adv. **6**, eaaz5015 (2020).

9. [†]Challenge of advanced low temperature fuel cells based on high degree of freedom of group 4 and 5 metal oxides: A. Ishihara, S. Tominaka, S. Mitsushima, H. Imai, O. Sugino and K.-I. Ota, Current Opinion in Electrochemistry **21**, 234 (2020).

10. [†]Completing density functional theory by machine learning hidden messages from molecules: R. Nagai, R. Akashi and O. Sugino, npj Comput Mater **6**, 43 (2020).

11. [†]Comparative Study on Sulfide and Oxide Electrolyte Interfaces with Cathodes in All-Solid-State Battery via First-Principles Calculations: Y. Okuno, J. Haruyama and Y. Tateyama, ACS Appl. Energy Mater. **3**, 11061 (2020).

12. [†]First-Principles Calculation of Copper Oxide Superconductors That Supports the Kamimura-Suwa Model: H. Kamimura, M. Araidai, K. Ishida, S. Matsuno, H. Sakata, K. Shiraishi, O. Sugino and J.-S. Tsai, Condensed Matter **5**, 69 (2020).

13. [†]*Ab initio* construction of the energy density functional for electron systems with the functional-renormalization-group-aided density functional theory: T. Yokota and T. Naito, Phys. Rev. Research **3**, L012015 (2021).

14. [†]Advances and challenges for experiment and theory for multi-electron multi-proton transfer at electrified solid-liquid interfaces: K. Sakaushi, T. Komeda, S. Hammes-Schiffer, M. M. Melander and O. Sugino, Phys. Chem. Chem. Phys. **22**, 19401-19442 (2021).

Oka group

The Oka group has constructed the theory for detecting Majorana modes in Kitaev's chiral spin liquid using STM setups. In addition, we have done a collaboration with experimentalists on novel transport properties in layered metals, as well as an High harmonics generation measurement in 3D Dirac materials.

1. h/e oscillations in interlayer transport of delafossites: C. Putzke, M. D. Bachmann, P. McGuinness, E. Zhakina, V. Sunko, M. Konczykowski, T. Oka, R. Moessner, A. Stern, M. König, S. Khim, A. P. Mackenzie and P. J. W. Moll, Science **368**, 1234 (2020).

2. Non-perturbative terahertz high-harmonic generation in the three-dimensional Dirac semimetal Cd_3As_2: S. Kovalev, R. M. Dantas, S. Germanskiy, J.-C. Deinert, B. Green, I. Ilyakov, N. Awari, M. Chen, M. Bawatna, J. Ling, F. Xiu, P. H. van Loosdrecht, P. Surówka, T. Oka and Z. Wang, Nature communications **11**, 1-6 (2020).

3. Scanning Tunneling Microscopy as a Single Majorana Detector of Kitaev's Chiral Spin Liquid: M. Udagawa, S. Takayoshi and T. Oka, Phys. Rev. Lett. **126**, 127201 (2021).

Inoue group

In 2020, we revealed a new family of light-driven inward H^+ pumping rhodopsin, schizorhodopsin (SzR), from Asgard archaea and marine micro-organisms. The mechanism of SzR was investigated by laser flash photolysis and FTIR spectroscopy. As the result, it was revealed that the H^+ of the retinal is released to the cytoplasmic milieu without being trapped at any amino acid residues in the protein. This is considerably different from that another inward H^+ pumping rhodopsin, xenorhodopsin. Also, we reported the role of a conserved tryptophan (Trp163) in the gating the mechanism of channelrhodopsin (C1C2). While the mutation of this residue (C1C2 W163F) reduced the channel activity, the H^+ pump activity was manifested.

1. Excitonic Coupling Effect on the Circular Dichroism Spectrum of Sodium-Pumping Rhodopsin KR2: K. J. Fujimoto and K. Inoue, J. Chem. Phys. **153**, 045101 (2020).

2. Allosteric Communication to the Retinal Chromophore upon Ion Binding in a Light-driven Sodium Ion Pumping Rhodopsin: A. Otomo, M. Mizuno, K. Inoue, H. Kandori and Y. Mizutani, Biochemistry **59**, 520-529 (2020).

3. Schizorhodopsins: A Novel Family of Rhodopsins from Asgard archaea that Function as Light-Driven Inward H^+ Pumps: K. Inoue, S. P. Tsunoda, M. Singh, S. Tomida, S. Hososhima, M. Konno, R. Nakamura, H. Watanabe, P. -A. Bulzu, H. L. Banciu, A. -S. Andrei, T. Uchihashi, R. Ghai, O. Béjà and H. Kandori, Sci. Adv. **6**, eaaz2441 (2020).

4. Infrared spectroscopic analysis on structural changes around the protonated Schiff base upon retinal isomerization in light-driven sodium pump KR2: S. Tomida, S. Ito, T. Mato, Y. Furutani, K. Inoue and H. Kandori, Biochimica et

[†] Joint research with outside partners.

Biophysica Acta (BBA) - Bioenergetics **1861**, 148190 (2020).

5. Physical disuse contributes to widespread chronic mechanical hyperalgesia, tactile allodynia, and cold allodynia through neurogenic inflammation and spino-parabrachio-amygdaloid pathway activation: Y. Ohmichi, M. Ohmichi, R. Tashima, K. Osuka, K. Fukushige, D. Kanikowska, Y. Fukazawa, H. Yawo, M. Tsuda, M. Naito and T. Nakano, PAIN **161**, 1808-1823 (2020).

6. Gate-keeper of ion transport – a highly conserved helix-3 tryptophan in a channelrhodopsin chimera, C1C2/ChRWR: Y. Nagasaka, S. Hososhima, N. Kubo, T. Nagata, H. Kandori, K. Inoue and H. Yawo, Biophys. Physicobiol. **17**, 59-69 (2020).

7. Active Learning for Level Set Estimation under Input Uncertainty and Its Extensions: Y. Inatsu, M. Karasuyama, K. Inoue and I. Takeuchi, Neural Computation **32**, 2486-2531 (2020).

8. Active Learning of Bayesian Linear Models with High-Dimensional Binary Features by Parameter Confidence-Region Estimation: Y. Inatsu, M. Karasuyama, K. Inoue, H. Kandori and I. Takeuchi, Neural Computation **32**, 1998-2031 (2020).

9. Crystal structure of schizorhodopsin reveals mechanism of inward proton pumping: A. Higuchi, W. Shihoya, M. Konno, T. Ikuta, H. Kandori, K. Inoue and O. Nureki, Proc. Natl. Acad. Sci. USA **118**, e2016328118 (2021).

10. Exploration of natural red-shifted rhodopsins using a machine learning-based Bayesian experimental design: K. Inoue, M. Karasuyama, R. Nakamura, M. Konno, D. Yamada, K. Mannen, T. Nagata, Y. Inatsu, H. Yawo, K. Yura, O. Béjà, H. Kandori and I. Takeuchi, Commun. Biol. **4**, 362 (2021).

11. TAT Rhodopsin Is an Ultraviolet-Dependent Environmental pH Sensor: C. Kataoka, T. Sugimoto, S. Shigemura, K. Katayama, S. P. Tsunoda, K. Inoue, O. Béjà and H. Kandori, Biochemistry, acs.biochem.0c00951 (2021), in print.

12. 光で細胞を制御する—多様な微生物型ロドプシンとオプトジェネティクス—: 井上 圭一 , 光学 **49**, 2-7 (2020).

13. Shining light on rhodopsin selectivity: How do proteins decide whether to transport H^+ or Cl^-?: K. Inoue, J. Biol. Chem. **295**, 14805-14806 (2020).

14. 光駆動タンパク質ロドプシンの分子機能エンジニアリング : 井上 圭一 , 生物工学会誌 **98**, 664-668 (2020).

15. ラットを用いたオプトジェネティクス（光遺伝学）: 八尾 寛 , 深澤 有吾 , 冨田 浩史 , 五十嵐 敬幸 , 日本実験動物協会情報誌　LABIO 21 **80**, 5-8 (2020).

16. A series of commentaries for a symposium entitled "Session 3SDA - Optogenetics: applying photoreceptor for understanding biological phenomena": S. P. Tsunoda and K. Inoue, Biophys Rev **12**, 295 (2020).

17. Expanding horizons of biosciences by light-control: M. Kataoka and T. Nagata, Biophysics and Physicobiology (2021), accepted for publication.

18. Application of Optogenetics for Muscle Cells and Stem Cells: T. Asano, D. B. L. Teh and H. Yawo, in: *Optogenetics*, edited by Hiromu Yawo, Hideki Kandori, Amane Koizumi, Ryoichiro Kageyama, (Springer Nature, 2021), 359-375.

19. Diversity, Mechanism, and Optogenetic Application of Light-Driven Ion Pump Rhodopsins: K. Inoue, in: *Optogenetics*, edited by Hiromu Yawo, Hideki Kandori, Amane Koizumi, Ryoichiro Kageyama, (Springer Nature, 2021), 89-126.

20. ロドプシンが拓くタンパク質科学の地平 : 井上 圭一 ,「未来探究２０５０　東大 30 人の知性が読み解く世界」, 東京大学未来ビジョン研究センター , (日本経済新聞出版 , 2021), 74-83.

Quantum Materials Group

Oshikawa group

We conducted theoretical studies on a wide range of subjects in quantum many-body problem. In particular, we proposed a novel mechanism of producing *robust* flat band in a network of conducting segments. In particular, in a honeycomb network, the flat band is stable as long as the hopping range is shorter than the segment length and the reflection symmetry of the honeycomb structure is kept. This may be realized in the nearly-commensurate charge density wave (NCCDW) phase of 1T-TaS_2, and could be a factor for the superconductivity observed at low temperatures in the vicinity of the NCCDW phase. We also introduced a new argument based on tilted boundary conditions for the Lieb-Schultz-Mattis (LSM) ingappability. It removes the need of an artificial restriction on system sizes, and elucidates the relation between the LSM ingappability in higher dimensions

[*] Joint research among groups within ISSP.

and the anomaly in quantum field theory in 1+1 dimensions.

1. †*Particle-Hole Symmetry Breaking in a Spin-Dimer System $TlCuCl_3$ Observed at 100 T: X. -G. Zhou, Y. Yao, Y. H. Matsuda, A. Ikeda, A. Matsuo, K. Kindo and H. Tanaka, Phys. Rev. Lett. **125**, 267207 1-6 (2020).

2. †Stable Flatbands, Topology, and Superconductivity of Magic Honeycomb Networks: J. M. Lee, C. Geng, J. W. Park, M. Oshikawa, S.-S. Lee, H. W. Yeom and G. Y. Cho, Phys. Rev. Lett. **124**, 137002 (2020).

3. Generalized Boundary Condition Applied to Lieb-Schultz-Mattis-Type Ingappabilities and Many-Body Chern Numbers: Y. Yao and M. Oshikawa, Phys. Rev. X **10**, 031008 (2020).

4. †Refined symmetry indicators for topological superconductors in all space groups: S. Ono, H. C. Po and H. Watanabe, Sci. Adv. **6**, eaaz8367 (1-14) (2020).

5. †Filling-enforced constraint on the quantized Hall conductivity on a periodic lattice: Y.-M. Lu, Y. Ran and M. Oshikawa, Annals of Physics **413**, 168060 (2020).

6. †Proof of the Absence of Long-Range Temporal Orders in Gibbs States: H. Watanabe, M. Oshikawa and T. Koma, J Stat Phys **178**, 926 (2020).

7. Non-local order parameters and quantum entanglement for fermionic topological field theories: K. Inamura, R. Kobayashi and S. Ryu, Journal of High Energy Physics **01**, 121(1-30) (2020).

8. Cyclotron resonance in Kondo insulator: Y. Tada, Physical Review Research **2**, 023194 (2020).

9. Quantum criticality of magnetic catalysis in two-dimensional correlated Dirac fermions: Y. Tada, Physical Review Research **2**, 033363 (2020).

10. Quantum valence bond ice theory for proton-driven quantum spin-dipole liquids: M. G. Yamada and Y. Tada, Physical Review Research **2**, 043077 (2020).

11. †Higher anomalies, higher symmetries, and cobordisms II: Lorentz symmetry extension and enriched bosonic / fermionic quantum gauge theory: Z. Wan, J. Wang and Y. Zheng, Annals of Mathematical Sciences and Applications **5**, 171 (2020).

12. †Non-Fermi Liquids in Conducting Two-Dimensional Networks: J. M. Lee, M. Oshikawa and G. Y. Cho, Phys. Rev. Lett. **126**, 186601 (2021).

13. †Parafermionization, bosonization, and critical parafermionic theories: Y. Yao and A. Furusaki, J. High Energ. Phys. **2021**, 285 (2021).

14. †Twisted boundary condition and Lieb-Schultz-Mattis ingappability for discrete symmetries: Y. Yao and M. Oshikawa, Phys. Rev. Lett. (2021), accepted for publication.

Nakatsuji group

A new era in quantum materials research arises, featuring discoveries of novel topological phases of matter and emergent quasiparticle excitations behaving as elusive elementary particles. Our research activities focus on designing and synthesizing new materials with emergent quantum properties that have never been seen before, then exploring the physics behind such properties with our world-leading measurement facilities. We aim to lead the innovative quest for new quantum materials that bear a far-reaching impact not only on basic science but also on our everyday life in the future. Major research themes: 1. Solid-state analogs of relativistic particles and new quantum phenomena · Weyl fermion and chiral anomaly · Quantum spin ice, magnetic monopole, and emergent photon 2. Room-temperature quantum transport phenomena in topological magnetic materials · Weyl antiferromagnets and their application to spintronic devices · Giant thermal and optical responses driven by the Berry curvature 3. Quantum phase transition in strongly correlated systems · Non-Fermi-liquid behavior and exotic superconductivity in multipolar Kondo materials

1. *Field-Orientation Effect on Ferro-Quadrupole Order in $PrTi_2Al_{20}$: S. Kittaka, T. Taniguchi, K. Hattori, S. Nakamura, T. Sakakibara, M. Takigawa, M. Tsujimoto, A. Sakai, Y. Matsumoto and S. Nakatsuji, J. Phys. Soc. Jpn. **89**, 043701(1-4) (2020).

2. Unveiling Quadrupolar Kondo Effect in the Heavy Fermion Superconductor PrV_2Al_{20}: M. Fu, A. Sakai, N. Sogabe, M. Tsujimoto, Y. Matsumoto and S. Nakatsuji, J. Phys. Soc. Jpn. **89**, 013704 (2020).

3. *Growth of $Pr_2Ir_2O_7$ thin films using solid phase epitaxy: T. Ohtsuki, Z. Tian, M. Halim, S. Nakatsuji and M. Lippmaa, J. Appl. Phys. **127**, 035303 (1-9) (2020).

† Joint research with outside partners.

4. Anomalous transverse response of Co_2MnGa and universality of the room-temperature ratio $\alpha_{ij}^{A}/\sigma_{ij}^{A}$ across topological magnets: L. Xu, X. Li, L. Ding, T. Chen, A. Sakai, B. Fauqué, S. Nakatsuji, Z. Zhu and K. Behnia, Phys. Rev. B **101**, 180404 (2020).

5. Antichiral spin order, its soft modes, and their hybridization with phonons in the topological semimetal Mn_3Ge: Y. Chen, J. Gaudet, S. Dasgupta, G. G. Marcus, J. Lin, T. Chen, T. Tomita, M. Ikhlas, Y. Zhao, W. C. Chen, M. B. Stone, O. Tchernyshyov, S. Nakatsuji and C. Broholm, Phys. Rev. B **102**, 054403 (2020).

6. Strong in-plane anisotropy in the electronic structure of fixed-valence β-$LuAlB_4$: P. Reiss, J. Baglo, H. Tan, X. Chen, S. Friedemann, K. Kuga, F. Malte Grosche, S. Nakatsuji and M. Sutherland, Phys. Rev. B **102**, 081102 (2020).

7. Impact of the lattice on magnetic properties and possible spin nematicity in the S = 1 triangular antiferromagnet $NiGa_2S_4$: M. E. Valentine, T. Higo, Y. Nambu, D. Chaudhuri, J. Wen, C. Broholm, S. Nakatsuji and N. Drichko, Phys. Rev. Lett. **125**, 197201 (2020).

8. Many-Body Resonance in a Correlated Topological Kagome Antiferromagnet: SS. Zhang, JX. Yin, M. Ikhlas, HJ. Tien, R. Wang, N. Shumiya, GQ. Chang, SS. Tsirkin, YG. Shi, CJ. Yi, Z. Guguchia, H. Li, WH. Wang, TR. Chang, ZQ. Wang, YF. Yang, T. Neupert, S. Nakatsuji and MZ. Hasan, Phys. Rev. Lett. **125**, 046401 (2020).

9. A tunable stress dilatometer and measurement of the thermal expansion under uniaxial stress of Mn_3Sn: M. Ikhlas, K. R. Shirer, P.-Y. Yang, A. P. Mackenzie, S. Nakatsuji and C. W. Hicks, Appl. Phys. Lett. **117**, 233502 (2020).

10. [*]Effect of sample size on anomalous Nernst effect in chiral antiferromagnetic Mn_3Sn devices: H. Narita, T. Higo, M. Ikhlas, S. Nakatsuji and Y. Otani, Appl. Phys. Lett. **116**, 072404 (2020).

11. [*]Magneto-optical Kerr effect in a non-collinear antiferromagnet Mn_3Ge: M. Wu, H. Isshiki, T. Chen, T. Higo, S. Nakatsuji and Y. Otani, Appl. Phys. Lett. **116**, 132408 (2020).

12. Superconducting properties of the ternary boride YRh_4B_4: J. Jatmika, H. Maruyama, M. S. Rahman, A. Sakai, S. Nakatsuji, A. Iyo and T. Ebihara, Supercond. Sci. Technol. **33**, 125006 (2020).

13. [*]Electrical manipulation of a topological antiferromagnetic state: H. Tsai, T. Higo, K. Kondou, T. Nomoto, A. Sakai, A. Kobayashi, T. Nakano, K. Yakushiji, R. Arita, S. Miwa, Y. Otani and S. Nakatsuji, Nature **580**, 608-613 (2020).

14. [*]Iron-based binary ferromagnets for transverse thermoelectric conversion: A. Sakai, S. Minami, T. Koretsune, T. Chen, T. Higo, Y. Wang, T. Nomoto, M. Hirayama, S. Miwa, D. Nishio-Hamane, F. Ishii, R. Arita and S. Nakatsuji, Nature **581**, 53-57 (2020).

15. 硬 X 線光電子分光と基礎物性測定により明らかにした価数の量子臨界現象：久我 健太郎 , 松本 洋介 , 大川 万里生 , 中辻 知 , 放射光 **33**, 1-8 (2020).

16. Magnetic and transport properties of amorphous, *B*2 and $L2_1$ Co_2MnGa thin films: Z. Zhu, T. Higo, S. Nakatsuji and Y. Otani, AIP Advances **10**, 085020 (2020).

17. [*]Structural and magnetic properties of Mn_3Ge films with Pt and Ru seed layers: A. Kobayashi, T. Higo, S. Nakatsuji and Y. Otani, AIP Advances **10**, 015225(1-6) (2020).

18. [*]Extracting the Chiral Contribution to the Negative Longitudinal Magnetoresistance in Epitaxial $Pr_2Ir_2O_7$ Thin Films: T. Ohtsuki, Z. Tian, A. Endo, M. Halim, S. Katsumoto, Y. Kohama, K. Kindo, M. Lippmaa and S. Nakatsuji, JPS Conf. Proc. **30**, 011181 (1-6) (2020).

19. [*]Magnetization and Thermal Expansion Properties of Quantum Spin Ice Candidate $Pr_2Zr_2O_7$: N. Tang, A. Sakai, K. Kimura, S. Nakamura, M. Fu, Y. Matsumoto, T. Sakakibara and S. Nakatsuji, JPS Conf. Proc. **30**, 011090(1-6) (2020).

20. Large Nernst Effect and Thermodynamics Properties in Weyl Antiferromagnet: T. Tomita, M. Ikhlas and S. Nakatsuji, JPS Conf. Proc **30**, 011009/1-7 (2020).

21. [*]Room-temperature terahertz anomalous Hall effect in Weyl antiferromagnet Mn_3Sn thin films: T. Matsuda, N. Kanda, T. Higo, N. P. Armitage, S. Nakatsuji and R. Matsunaga, Nat Commun **11**, 909 (2020).

22. [*]Electrical nucleation, displacement, and detection of antiferromagnetic domain walls in the chiral antiferromagnet Mn_3Sn: S. Sugimoto, Y. Nakatani, Y. Yamane, M. Ikhlas, K. Kondou, M. Kimata, T. Tomita, S. Nakatsuji and Y. Otani, Commun Phys **3**, 111 (2020).

23. Sample Quality Dependence of the Magnetic Properties in Non-Collinear Antiferromagnet Mn_3Sn: M. Ikhlas, T. Tomita and S. Nakatsuji, JPS. Conf. Proc **30**, 011177 (2020).

---

[*] Joint research among groups within ISSP.

24. Crystal structure and magnetic properties of the ferromagnet CoMnSb: H. Nakamura, M. Y. P. Akbar, T. Tomita, A. A. Nugroho and S. Nakatsuji, JPS Conference Proceedings **29**, 013004/1-5 (2020).

25. Unconventional free charge in the correlated semimetal $Nd_2Ir_2O_7$: K. Wang, B. Xu, C. W. Rischau, N. Bachar, B. Michon, J. Teyssier, Y. Qiu, T. Ohtsuki, B. Cheng, N. P. Armitage, S. Nakatsuji and D. van der Marel, Nat. Phys. **16**, 1194–1198 (2020).

26. Superconducting properties of the ternary boride YRh_4B_4: J. Jatmika, H. Maruyama, MS. Rahman, A. Sakai, S. Nakatsuji, A. Iyo and T. Ebihara, SUPERCONDUCTOR SCIENCE & TECHNOLOGY, **33**, 125006 (2020).

27. *Low Gilbert damping in the nodal-line semimetal $D0_3$-Fe_3Ga epitaxial thin film: S. Sakamoto, T. Higo, S. Tamaru, H. Kubota, K. Yakushiji, S. Nakatsuji and S. Miwa, Phys. Rev. B **103**, 165122 (1-5) (2021).

28. *Domain structure and domain wall dynamics in topological chiral antiferromagnets from the viewpoint of magnetic octupole: Y. Otani and T. Higo, Appl. Phys. Lett. **118**, 040501 (2021).

29. *Omnidirectional Control of Large Electrical Output in a Topological Antiferromagnet: T. Higo, Y. Li, K. Kondou, D. Qu, M. Ikhlas, R. Uesugi, D. Nishio-Hamane, C. L. Chien, Y. Otani and S. Nakatsuji, Adv. Funct. Mater. **31**, 2008971-12 (2021).

30. *Spin-orbit torque switching of the antiferromagnetic state in polycrystalline Mn_3Sn/Cu/heavy metal heterostructures: H. Tsai, T. Higo, K. Kondou, A. Kobayashi, T. Nakano, K. Yakushiji, S. Miwa, Y. Otani and S. Nakatsuji, AIP Advances **11**, 045110 (1-6) (2021).

31. Anomalous transport due to Weyl fermions in the chiral antiferromagnets Mn_3X, X=Sn, Ge: T. Chen, T. Tomita, S. Minami, M. Fu, T. Koretsune, M. Kitatani, I. Muhammad, D. Nishio-Hamane, R. Ishii, F. Ishii, R. Arita and S. Nakatsuji, Nat. Commun. **12**, 572 (2021).

32. Inhomogeneous Kondo-lattice in geometrically frustrated $Pr_2Ir_2O_7$: M. Kavai, J. Friedman, K. Sherman, M. Gong, I. Giannakis, S. Hajinazar, H. Hu, S. E. Grefe, J. Leshen, Q. Yang, S. Nakatsuji, A. N. Kolmogorov, Q. Si, M. Lawler and P. Aynajian, Nat. Commun. **12**, 1377 (2021).

33. *Fabrication of polycrystalline Weyl antiferromagnetic Mn_3Sn thin films on various seed layers: T. Nakano, T. Higo, A. Kobayashi, S. Miwa, S. Nakatsuji and K. Yakushiji, Phys. Rev. Materials **5**, 054402 (1-9) (2021).

34. *Giant Effective Damping of Octupole Oscillation in an Antiferromagnetic Weyl Semimetal: S. Miwa, S. Iihama, T. Nomoto, T. Tomita, T. Higo, M. Ikhlas, S. Sakamoto, Y. Otani, S. Mizukami, R. Arita and S. Nakatsuji, Small Science **1**, 2000062 (1-8) (2021).

35. *Large Hall Signal due to Electrical Switching of an Antiferromagnetic Weyl Semimetal State: H. Tsai, T. Higo, K. Kondou, S. Sakamoto, A. Kobayashi, T. Matsuo, S. Miwa, Y. Otani and S. Nakatsuji, Small Science **1**, 2000025 (1-9) (2021).

Miwa group

We have studied the following topics this year: (1) Spin-torque effect on a chiral antiferromagnet Mn_3Sn, (2) Thin film growth of a line-node ferromagnet Fe3X, and (3) Chiral molecular spintronics device. In topic (1), we find that it is feasible to control a topological antiferromagnetic state in Mn_3Sn by using an unconventional spin-transfer effect (Nature 580, 608). This is a work in collaboration with Nakatsuji and Otani groups. In topic (2), we have succeeded in preparing Fe_3Al and Fe_3Gd thin film by using a molecular beam epitaxy method, which shows giant anomalous Nernst effect as those in a bulk form (Nature 581, 53). This is a work in collaboration with Nakatsuji group. In topic (3), we find a chirality-induced effective magnetic field in a phthalocyanine molecule at Fe/MgO interface. Unlike the previous study, our system shows an effective magnetic field in the absence of a bias current in the system (Appl. Phys. Express 13, 113001, Spotlights 2020).

1. Voltage-controlled magnetic anisotropy in an ultrathin nickel film studied by operando x-ray magnetic circular dichroism spectroscopy: R. Miyakaze, S. Sakamoto, T. Kawabe, T. Tsukahara, Y. Kotani, K. Toyoki, T. Nakamura, M. Goto, Y. Suzuki and S. Miwa, Phys. Rev. B **102**, 014419 (1-6) (2020).

2. Investigation of gating effect in Si spin MOSFET: S. Lee, F. Rortais, R. Ohshima, Y. Ando, M. Goto, S. Miwa, Y. Suzuki, H. Koike and M. Shiraishi, Appl. Phys. Lett. **116**, 022403 (1-5) (2020).

3. Sizable spin-transfer torque in the Bi/$Ni_{80}Fe_{20}$ bilayer film: M. Matsushima, S. Miwa, S. Sakamoto, T. Shinjo, R. Ohshima, Y. Ando, Y. Fuseya and M. Shiraishi, Appl. Phys. Lett. **117**, 042407 (1-4) (2020).

4. *Electrical manipulation of a topological antiferromagnetic state: H. Tsai, T. Higo, K. Kondou, T. Nomoto, A. Sakai, A. Kobayashi, T. Nakano, K. Yakushiji, R. Arita, S. Miwa, Y. Otani and S. Nakatsuji, Nature **580**, 608-613 (2020).

† Joint research with outside partners.

5. *Iron-based binary ferromagnets for transverse thermoelectric conversion: A. Sakai, S. Minami, T. Koretsune, T. Chen, T. Higo, Y. Wang, T. Nomoto, M. Hirayama, S. Miwa, D. Nishio-Hamane, F. Ishii, R. Arita and S. Nakatsuji, Nature **581**, 53-57 (2020).

6. Control of Spin–Orbit Torques by Interface Engineering in Topological Insulator Heterostructures: F. Bonell, M. Goto, G. Sauthier, J. F. Sierra, A. I. Figueroa, M. V. Costache, S. Miwa, Y. Suzuki and S. O. Valenzuela, Nano Lett. **20**, 5893-5899 (2020).

7. Detection of Spin Transfer from Metal to Molecule by Magnetoresistance Measurement: H. Gamou, K. Shimose, R. Enoki, E. Minamitani, A. Shiotari, Y. Kotani, K. Toyoki, T. Nakamura, Y. Sugimoto, M. Kohda, J. Nitta and S. Miwa, Nano Lett. **20**, 75-80 (2020).

8. *Chirality-induced effective magnetic field in a phthalocyanine molecule: S. Miwa, K. Kondou, S. Sakamoto, A. Nihonyanagi, F. Araoka, Y. Otani and D. Miyajima, Appl. Phys. Express **13**, 113001 (1-4) (Spotlights 2020) (2020).

9. Over 1% magnetoresistance ratio at room temperature in non-degenerate silicon-based lateral spin valves: H. Koike, S. Lee, R. Ohshima, E. Shigematsu, M. Goto, S. Miwa, Y. Suzuki, T. Sasaki, Y. Ando and M. Shiraishi, Appl. Phys. Express **13**, 083002 (1-4) (2020).

10. Enhancement of spin signals by thermal annealing in silicon-based lateral spin valves: N. Yamashita, S. Lee, R. Ohshima, E. Shigematsu, H. Koike, Y. Suzuki, S. Miwa, M. Goto, Y. Ando and M. Shiraishi, AIP Advances **10**, 095021 (1-6) (2020).

11. Electrical Control for Extending the Ramsey Spin Coherence Time of Ion-Implanted Nitrogen-Vacancy Centers in Diamond: S. Kobayashi, Y. Matsuzaki, H. Morishita, S. Miwa, Y. Suzuki, M. Fujiwara and N. Mizuochi, Phys. Rev. Applied **14**, 044033 (1-10) (2020).

12. Gate-Tunable Spin XOR Operation in a Silicon-Based Device at Room Temperature: R. Ishihara, Y. Ando, S. Lee, R. Ohshima, M. Goto, S. Miwa, Y. Suzuki, H. Koike and M. Shiraishi, Phys. Rev. Applied **13**, 044010 (1-9) (2020).

13. *Low Gilbert damping in the nodal-line semimetal $D0_3$-Fe_3Ga epitaxial thin film: S. Sakamoto, T. Higo, S. Tamaru, H. Kubota, K. Yakushiji, S. Nakatsuji and S. Miwa, Phys. Rev. B **103**, 165122 (1-5) (2021).

14. Physically Unclonable Functions With Voltage-Controlled Magnetic Tunnel Junctions: Y. Tanaka, M. Goto, A. K. Shukla, K. Yoshikawa, H. Nomura, S. Miwa, S. Tomishima and Y. Suzuki, IEEE Trans. Magn. **57**, 3400806 (1-6) (2021).

15. *Spin-orbit torque switching of the antiferromagnetic state in polycrystalline Mn_3Sn/Cu/heavy metal heterostructures: H. Tsai, T. Higo, K. Kondou, A. Kobayashi, T. Nakano, K. Yakushiji, S. Miwa, Y. Otani and S. Nakatsuji, AIP Advances **11**, 045110 (1-6) (2021).

16. *Fabrication of polycrystalline Weyl antiferromagnetic Mn_3Sn thin films on various seed layers: T. Nakano, T. Higo, A. Kobayashi, S. Miwa, S. Nakatsuji and K. Yakushiji, Phys. Rev. Materials **5**, 054402 (1-9) (2021).

17. *Giant Effective Damping of Octupole Oscillation in an Antiferromagnetic Weyl Semimetal: S. Miwa, S. Iihama, T. Nomoto, T. Tomita, T. Higo, M. Ikhlas, S. Sakamoto, Y. Otani, S. Mizukami, R. Arita and S. Nakatsuji, Small Science **1**, 2000062 (1-8) (2021).

18. *Large Hall Signal due to Electrical Switching of an Antiferromagnetic Weyl Semimetal State: H. Tsai, T. Higo, K. Kondou, S. Sakamoto, A. Kobayashi, T. Matsuo, S. Miwa, Y. Otani and S. Nakatsuji, Small Science **1**, 2000025 (1-9) (2021).

19. 電圧トルク MRAM に向けた新材料探索と磁化反転制御技術開発 : 野崎 隆行 , 山本 竜也 , 三輪 真嗣 , 鈴木 義茂 , 湯浅 新治 , まぐね **15**, 15-23 (2020).

20. 磁気抵抗効果を使ったスピントロニクス現象 : 三輪 真嗣 , 電気評論 **105**, 21-28 (2020).

Division of Data-Integrated Materials Science

Fukushima group

We have developed an automatic exhaustive calculation tool which is based on the Korriga-Kohn-Rostoker coherent potential approximation (KKR-CPA) method. Our tool can explore the huge materials space consisting of disordered systems and construct large-scale materials databases. In this year, we implemented new features in our tool. One is the scale-bridging

* Joint research among groups within ISSP.

(multi-scale) simulation technique combining KKR-CPA and Monte Carlo methods for magnetocaloric materials. We applied this method to MnCoGe alloys systems and succeeded in quantitatively evaluating the Curie temperature, magnetic entropy, and isothermal entropy. Another is the calculation technique of electronic structures, magnetic properties, and transport properties at finite temperature. Temperature effects often have a significant influence on the materials properties. To investigate the electronic structures at finite temperature, we need to incorporate the effects of local phonon excitations and spin-wave (magnon) excitations in the framework of the KKR-CPA method. In the KKR Green's function method, the single-site t-matrix is the sum of the coefficients of partial wave expansion at each atomic position and contains information of the single-site scattering effect. We can thus replace the multiple scattering effect by an effective medium potential using CPA. The local phonon excitation and magnon excitation can be treated as as the configuration average with respect to the local phonon displacements and local moment disorder (LMD) states, respectively. We performed KKR-CPA calculations of temperature-dependent electronic structures and transport properties of the half-metallic Heusler alloy Co_2MnSi. The electrical resistivity was calculated by the Kubo-Greenwood formula. For Co_2MnSi, due to impurity scattering by the Mn-Co antisite disorder, a rather large residual resistivity exists. Hundling the local phonon, magnon, and Mn-Co antisite disorders simultaneously by CPA, we were able to reproduce the experimentally observed temperature-dependent resistivity. Thus, we not only calculated the electronic structures incorporating temperature effects, which are difficult for conventional first-principles approaches, but also estimated the transport properties of the half-metallic Heusler alloy. Our method replicated the experiments and was demonstrated to be effective. Applying this method to other Heusler alloys and superlattices with giant magnetoresistance (GMR) and TMR structures, it will be possible to exploit theoretically-driven materials design of next-generation spintronics.

1. Hole-mediated ferromagnetism in a high-magnetic moment material, Gd-doped GaN: A. Masago, H. Shinya, T. Fukushima, K. Sato and H. Katayama-Yoshida, J. Phys.: Condens. Matter **32**, 485803(1-6) (2020).

2. Magnetocaloric effect in MnCoGe alloys studied by first-principles calculations and Monte-Carlo simulation: H. B. Tran, T. Fukushima, Y. Makino and T. Oguchi, Solid State Commun. **323**, 114077(1-5) (2020).

3. *First-principles calculations of finite temperature electronic structures and transport properties of Heusler alloy Co_2MnSi: H. Shinya, S. Kou, T. Fukushima, A. Masago, K. Sato, H. Katayama-Yoshida and H. Akai, Appl. Phys. Lett. **117**, 042402(1-5) (2020).

4. Tuning structural-transformation temperature toward giantmagnetocaloric effect in MnCoGe alloy: A theoretical study: H. B. Tran, T. Fukushima, K. Sato, Y. Makino and T. Oguchi, J. Alloys Compd. **854**, 157063(1-9) (2020).

5. Spin injection through energy-band symmetry matching with high spin polarization in atomically controlled ferromagnet/ferromagnet/ semiconductor structures: M. Yamada, F. Kuroda, M. Tsukahara, S. Yamada, T. Fukushima, K. Sawano, T. Oguchi and K. Hamaya, NPG Asia Mater. **12**, 47(1-9) (2020).

6. Valence states and the magnetism of Eu ions in Eu-doped GaN: T. Nunokawa, Y. Fujiwara, Y. Miyata, N. Fujimura, T. Sakurai, H. Ohta, A. Masago, H. Shinya, T. Fukushima, K. Sato and H. Katayama-Yoshida, J. Appl. Phys **127**, 083901(1-7) (2020).

7. High Curie temperature in Eu-doped GaN caused by volume-compensated Ga-vacancy: A. Masago, H. Shinya, T. Fukushima, K. Sato and H. Katayama-Yoshida, AIP Adv. **10**, 025216(1-4) (2020).

8. First-principles calculation of electronic density of states and Seebeck coefficient in transition-metal-doped Si–Ge alloys: R. Yamada, A. Masago, T. Fukushima, H. Shinya, T. Q. Nguyen and K. Sato, Solid State Commun. **323**, 110227(1-8) (2021).

9. Effect of atomic configuration on magnetic properties and electronicstate of CoVMnAl quaternary heusler alloy: R. Y. Umetsu, K. Saito, K. Ono, T. Fukushima, F. Kuroda, T. Oguchi and T. Ishigaki, J. Alloys Compd. **855**, 157389(1-9) (2021).

10. Theoretical prediction of large anisotropic magnetocaloric effect in MnP: H. B. Tran, T. Fukushima, H. Momida, K. Sato, Y. Makino and T. Oguchi, Comput. Mater. Sci. **188**, 110227(1-8) (2021).

11. Intrinsic defect formation and the effect of transition metal doping on transport properties in a ductile thermoelectric material α-Ag_2S: a first-principles study: H. N. Nam, R. Yamada, H. Okumura, T. Q. Nguyen, K. Suzuki, H. Shinya, A. Masago, T. Fukushima and K. Sato, Phys. Chem. Chem. Phys (2021), accepted for publication.

† Joint research with outside partners.

Materials Design and Characterization Laboratory

Hiroi group

A new titanium hydride complex $BaCa_2Ti_2H_{14}$ with the 9-fold coordination was discovered. A new spin-orbit-coupled metal candidate $PbRe_2O_6$ was studied. Kitaev spin liquid candidate Os_xCl_3 comprised of honeycomb nano-domains was investigated. A multipolar order in the spin-orbit-coupled 5d Mott insulator B_2MgReO_6 was studied by high-resolution XRD.

1. *Domain Control by Adjusting Anisotropic Stress in Pyrochlore Oxide $Cd_2Re_2O_7$: S. Tajima, D. Hirai, Y. Kinoshita, M. Tokunaga, K. Akiba, T. C. Kobayashi, H. T. Hirose and Z. Hiroi, J. Phys. Soc. Jpn. **89**, 114711 (2020).

2. *Kitaev Spin Liquid Candidate Os_xCl_3 Comprised of Honeycomb Nano-Domains: K. Kataoka, D. Hirai, T. Yajima, D. Nishio-Hamane, R. Ishii, K.-Y. Choi, D. Wulferding, P. Lemmens, S. Kittaka, T. Sakakibara, H. Ishikawa, A. Matsuo, K. Kindo and Z. Hiroi, J. Phys. Soc. Jpn. **89**, 114709(1-9) (2020).

3. Variation in Superconducting Symmetry Against Pressure on Noncentrosymmetric Superconductor $Cd_2Re_2O_7$ Revealed by 185/187Re Nuclear Quadrupole Resonance: S. Kitagawa, K. Ishida, T. C. Kobayashi, Y. Matsubayashi, D. Hirai and Z. Hiroi, J. Phys. Soc. Jpn. **89**, 053701 (2020).

4. Anomalous changes of electric quadrupole order at low temperatures in the spin-orbit coupled metal $Cd_2Re_2O_7$: S. Uji, S. Sugiura, H. T. Hirose, T. Terashima, Y. Matsubayashi, D. Hirai, Z. Hiroi and T. Hasegawa, Phys. Rev. B **102**, 155131 (2020).

5. Antiferromagnetic long-range order in the 5d(1) double-perovskite Sr_2MgReO_6: S. Gao, D. Hirai, H. Sagayama, H. Ohsumi, Z. Hiroi and T.-H. Arima, Phys. Rev. B **101**, 220412 (2020).

6. Coexistence of odd-parity and even-parity order parameters in the multipole order phase of the spin-orbit coupled metal $Cd_2Re_2O_7$: Y. Matsubayashi, K. Sugii, D. Hirai, Z. Hiroi, T. Hasegawa, S. Sugiura, H. T. Hirose, T. Terashima and S. Uji, Phys. Rev. B **101**, 205133 (2020).

7. *Helical and collinear spin density wave order in the S = 1/2 one-dimensional frustrated chain compound NaCuMoO4(OH) investigated by neutron scattering: S. Asai, T. Oyama, K. Nawa, A. Nakao, K. Munakata, K. Kuwahara, M. Hagihala, S. Itoh, Z. Hiroi and T. Masuda, Phys. Rev. B **101**, 144437(1-8) (2020).

8. *Zero-energy excitation in the classical kagome antiferromagnet $NaBa_2Mn_3F_{11}$: S. Hayashida, H. Ishikawa, Y. Okamoto, T. Okubo, Z. Hiroi, G. J. Nilsen, H. Mutka and T. Masuda, Phys. Rev. B **101**, 214409 (2020).

9. *Anisotropic Triangular Lattice Realized in Rhenium Oxychlorides $A_3ReO_5Cl_2$ (A = Ba, Sr): D. Hirai, T. Yajima, K. Nawa, M. Kawamura and Z. Hiroi, Inorg. Chem. **59**, 10025 (2020).

10. Titanium Hydride Complex $BaCa_2Ti_2H_{14}$ with 9-Fold Coordination: T. Yajima, H. Nakajima, T. Honda, K. Ikeda, T. Otomo, H. Takeda and Z. Hiroi, Inorg. Chem. **59**, 4228 (2020).

11. *Spin–orbit-coupled metal candidate $PbRe_2O_6$: S. Tajima, D. Hirai, T. Yajima, D. Nishio-Hamane, Y. Matsubayashi and Z. Hiroi, Journal of Solid State Chemistry **288**, 121359 (2020).

12. *Thermal Hall Effects of Spins and Phonons in Kagome Antiferromagnet Cd-Kapellasite: M. Akazawa, M. Shimozawa, S. Kittaka, T. Sakakibara, R. Okuma, Z. Hiroi, H.-Y. Lee, N. Kawashima, J. H. Han and M. Yamashita, Phys. Rev. X **10**, 041059 (2020).

13. Detection of multipolar orders in the spin-orbit-coupled 5*d* Mott insulator B_2MgReO_6: D. Hirai, H. Sagayama, S. Gao, H. Ohsumi, G. Chen, T.-H. Arima and Z. Hiroi, Phys. Rev. Research **2**, 022063 (2020).

14. †**Single shot x-ray diffractometry in SACLA with pulsed magnetic fields up to 16 T: A. Ikeda, Y. H. Matsuda, X. Zhou, T. Yajima, Y. Kubota, K. Tono and M. Yabashi, Phys. Rev. Research **2**, 043175 1-6 (2020).

15. *Pressure-induced phase transition in the J_1-J_2 square lattice antiferromagnet $RbMoOPO_4Cl$: H. Takeda, T. Yamauchi, M. Takigawa, H. Ishikawa and Z. Hiroi, Phys. Rev. B **103**, 104406 (2021).

Kawashima group

We developed highly efficient methods, algorithms, and parallelized programs based on the tensor network (TN) method and applied them to relevant physical problems, which include the following: (1) development of decomposition method of a high-ranked tensor into a ring of smaller low-ranked tensors, (2) development of TN method for boundary phenomena, (3) study of Kitaev spin liquid by TN variational functions, (4) study of spin liquid in frustrated spin systems, (5) TN study of deconfined-critical phenomena, and (6) TN implementation of rael-space renormalization group.

---

* Joint research among groups within ISSP.

1. Frustration-induced supersolid phases of extended Bose–Hubbard model in the hard-core limit: W.-L. Tu, H.-K. Wu and T. Suzuki, J. Phys.: Condens. Matter **32**, 455401 (2020).
2. Tensor-Ring Decomposition with Index-Splitting: H.-Y. Lee and N. Kawashima, J. Phys. Soc. Jpn. **89**, 054003(1-9) (2020).
3. Abelian and non-Abelian chiral spin liquids in a compact tensor network: H.-Y. Lee, R. Kaneko, T. Okubo and N. Kawashima, Phys. Rev. B **101**, 035140 (2020).
4. Boundary conformal spectrum and surface critical behavior of classical spin systems:A tensor network renormalization study: S. Iino, S. Morita and N. Kawashima, Phys. Rev. B **101**, 155418 (2020).
5. Construction of variational matrix product states for the Heisenberg spin-1 chain: J. Kim, M. Kim, N. Kawashima, J. H. Han and H.-Y. Lee, Phys. Rev. B **102**, 085117(1-8) (2020).
6. Competing quantum phases of hard-core bosons with tilted dipole-dipole interaction: H.-K. Wu and W.-L. Tu, Phys. Rev. A **102**, 053306 (2020).
7. *Thermal Hall Effects of Spins and Phonons in Kagome Antiferromagnet Cd-Kapellasite: M. Akazawa, M. Shimozawa, S. Kittaka, T. Sakakibara, R. Okuma, Z. Hiroi, H.-Y. Lee, N. Kawashima, J. H. Han and M. Yamashita, Phys. Rev. X **10**, 041059 (2020).
8. Magnetic field induced quantum phases in a tensor network study of Kitaev magnets: H.-Y. Lee, R. Kaneko, L. E. Chern, T. Okubo, Y. Yamaji, N. Kawashima and Y. B. Kim, Nature Communications **11**, 1639 (2020).
9. Magnetic field induced competing phases in spin-orbital entangled Kitaev magnets: L. E. Chern, R. Kaneko, H.-Y. Lee and Y. B. Kim, Phys. Rev. Research **2**, 013014 (2020).
10. Tensor network wave function of S=1 Kitaev spin liquids: H.-Y. Lee, N. Kawashima and Y. B. Kim, Phys. Rev. Research **2**, 033318(1-6) (2020).
11. * 分子動力学計算による複雑流体中のカルマン渦の解析：浅野 優太 , 渡辺 宙志 , 野口 博司 , 分子シミュレーション学会誌 " アンサンブル " **22**, 157-162 (2020).
12. Effective Ruderman–Kittel–Kasuya–Yosida-like Interaction in Diluted Double-exchange Model: Self-learning Monte Carlo Approach: H. Kohshiro and Y. Nagai, J. Phys. Soc. Jpn. **90**, 034711 (2021).
13. Continuous phase transition between Neel and valence bond solid phases in a J-Q-like spin ladder system: T. Ogino, R. Kaneko, S. Morita, S. Furukawa and N. Kawashima, Phys. Rev. B **103**, 085117 (2021).
14. Global optimization of tensor renormalization group using the corner transfer matrix: S. Morita and N. Kawashima, Phys. Rev. B **103**, 045131(1-6) (2021).
15. †*DSQSS: Discrete Space Quantum Systems Solver: Y. Motoyama, K. Yoshimi, A. Masaki-Kato, T. Kato and N. Kawashima, Computer Physics Communications **264**, 107944 (2021).
16. †*Kω— Open-source library for the shifted Krylov subspace method of the form $(zI - H)x = b$: T. Hoshi, M. Kawamura, K. Yoshimi, Y. Motoyama, T. Misawa, Y. Yamaji, S. Todo, N. Kawashima and T. Sogabe, Computer Physics Communications **258**, 107536 (2021).
17. "Data Assimilation Method for Experimental and First-Principles Data: Finite-Temperature Magnetization of $(Nd,Pr,La,Ce)_2(Fe,Co,Ni)_{14}B$": Y. Harashima, K. Tamai, S. Doi, M. Matsumoto, H. Akai, N. Kawashima, M. Ito, N. Sakuma, A. Kato, T. Shoji and T. Miyake, Phys. Rev. Materials **5**, 013806(1-10) (2021).
18. Scaling dimensions from linearized tensor renormalization group transformations: X. Lyu, R. G. Xu and N. Kawashima, Phys. Rev. Research **3**, 023048 (2021).
19. Boundary CFT and Tensor Network Approach to Surface Critical Phenomena of the Tricritical 3-State Potts model: S. Iino, J Stat Phys **182**, 56 (2021).
20. DSQSS: Discrete Space Quantum Systems Solver: Y. Motoyama, K. Yoshimi, A. Masaki-Kato, T. Kato and N. Kawashima, Computer Physics Communications **264**, 107944 (2021), accepted for publication.

Uwatoko group

The effect of pressure on the unique electronic state of the antiferromagnetic (AF) compound $EuCu_2Ge_2$ has been measured in a wide temperature range from 10 mK to 300 K by electrical resistivity measurements up to 10 GPa. The results exhibit that

† Joint research with outside partners.

critical pressure, ~6.5 GPa, coincides with valence transition pressure, corresponding to the quantum criticality of the valence transition. A "palm" cubic-anvil pressure cell (PCAC) having an outer diameter of 60 mm, the smallest cubic-anvil cell to date, was fabricated to physical measurements with superconducting magnet. The PCAC is advantageous because a large sample space and pressure homogeneity are secured even under frozen pressure media environment at high pressures. We investigate the pressure effect on the large anomalous Hall effect (AHE) of $Co_3Sn_2S_2$ up to 12 GPa with a palm cubic anvil cell apparatus and first-principles calculations simulation. We find that both the ferromagnetic transition temperature and the AHE are suppressed monotonically upon the application of high pressure. Combined with theoretical calculations, our results indicate that the distance between Weyl points with opposite chirality in $Co_3Sn_2S_2$ is substantially reduced accompanying the suppression of ferromagnetism by pressure, thus providing an experimental route to tune the AHE of magnetic Weyl semimetals via modifying the nontrivial band topology.

1. Pressure effect on the magnetoresistivity of topological semimetal RhSn: S. Xu, S. Xu, J. Sun, B. Wang, Y. Uwatoko, T. Xia and J. Cheng, J. Phys.: Condens. Matter **32**, 355601(1-6) (2020).

2. Magnetoelectric Effect in the Antiferromagnetic Ordered State of Ce_3TiBi_5 with Ce Zig-Zag Chains: M. Shinozaki, G. Motoyama, M. Tsubouchi, M. Sezaki, J. Gouchi, S. Nishigori, T. Mutou, A. Yamaguchi, K. Fujiwara, K. Miyoshi and Y. Uwatoko, J. Phys. Soc. Jpn. **89**, 033703(1-5) (2020).

3. Quantum Criticality of Valence Transition for the Unique Electronic State of Antiferromagnetic Compound $EuCu_2Ge_2$: J. Gouchi, K. Miyake, W. Iha, M. Hedo, T. Nakama, Y. Ônuki and Y. Uwatoko, J. Phys. Soc. Jpn. **89**, 053703(1-5) (2020).

4. Single-Crystal Growth and Physical Properties of $EuZn_2Ge_2$: M. Kosaka, S. Michimura, H. Hirabayashi, R. Numakura, R. Iizuka, K. Kuwahara and Y. Uwatoko, J. Phys. Soc. Jpn. **89**, 054704(1-8) (2020).

5. Coupled magnetic and structural phase transitions in the antiferromagnetic polar metal Pb_2CoOsO_6 under pressure: Y. Jiao, Y.-W. Fang, J. Sun, P. Shan, Z. Yu, H. L. Feng, B. Wang, H. Ma, Y. Uwatoko, K. Yamaura, Y. Guo, H. Chen and J. Cheng, Phys. Rev. B **102**, 144418(1-7) (2020).

6. High pressure investigation of an organic three-dimensional Dirac semimetal candidate having a diamond lattice: A. Kiswandhi, M. Maesato, S. Tomeno, Y. Yoshida, Y. Shimizu, P. Shahi, J. Gouchi, Y. Uwatoko, G. Saito and H. Kitagawa, Phys. Rev. B **101**, 245124(1-7) (2020).

7. *Magnetotransport properties of tellurium under extreme conditions: K. Akiba, K. Kobayashi, T. C. Kobayashi, R. Koezuka, A. Miyake, J. Gouchi, Y. Uwatoko and M. Tokunaga, Phys. Rev. B **101**, 245111(1-6) (2020).

8. Physical properties and pressure-induced superconductivity in the single-crystalline band insulator SnO: S. Xu, Y. Zou, J. Sun, Z. Liu, X. Yu, J. Gouchi, Y. Uwatoko, Z. G. Cheng, B. Wang and J. Cheng, Phys. Rev. B **101**, 104501(1-8) (2020).

9. Pressure-induced incommensurate antiferromagnetic order in a ferromagnetic B-site ordered double-perovskite Lu_2NiMnO_6: N. Terada, C. V. Colin, N. Qureshi, T. C. Hansen, K. Matsubayashi, Y. Uwatoko and A. A. Belik, Phys. Rev. B **102**, 094412(1-9) (2020).

10. *Sample dependence of half-integer quantized thermal Hall effect in the Kitaev spin-liquid candidate α-$RuCl_3$: M. Yamashita, J. Gouchi, Y. Uwatoko, N. Kurita and H. Tanaka, Phys. Rev. B **102**, 220404(R) (2020).

11. Superconducting phase diagrams of S-doped 2*H*−$TaSe_2$ under hydrostatic pressure: S. Xu, Z. Liu, P. Yang, K. Chen, J. Sun, J. Dai, Y. Yin, F. Hong, X. Yu, M. Xue, J. Gouchi, Y. Uwatoko, B. Wang and J. Cheng, Phys. Rev. B **102**, 184511(1-9) (2020).

12. Weak ferromagnetism and possible non-Fermi-liquid behavior in the itinerant electronic material Co_3SnC: B. Wang, Y. Uwatoko, J. Cheng and Y. Sun, Phys. Rev. B **102**, 085153(1-9) (2020).

13. NMR study under pressure on the iron-based superconductor $FeSe_{1-x}S_x$ (x = 0.12 and 0.23): Relationship between nematicity and AF fluctuations: T. Kuwayama, K. Matsuura, Y. Mizukami, S. Kasahara, Y. Matsuda, T. Shibauchi, Y. Uwatoko and N. Fujiwara, Mod. Phys. Lett. B **34**, 2040048(1-6) (2020).

14. Effects of Substituted Elements on Spin Reorientation in $Mn_{2-x}Fe_xSb_{1-y}Sn_y$: K. Noguchi, Y. Mitsui, M. Hiroi, R. Y. Umetsu, J. Gouchi, Y. Uwatoko and K. Koyama, Mater. Trans. **61**, 1492-1495 (2020).

15. Magnetic Field Effect on Nitrogenation of Sm_2Fe_{17}: K. Koyama, M. Onoue, R. Kobayashi, Y. Mitsui, R. Y. Umetsu and Y. Uwatoko, Mater. Trans. **61**, 1487-1491 (2020).

16. Magnetic Measurements of Narrow-Gap Semiconductor $FeSb_2$ under High Pressure: T. Deguchi, K. Matsubayashi, Y. Uwatoko, T. Koyama, T. Kohara, H. Nakamura, Y. Mitsui and K. Koyama, Mater. Trans. **61**, 1476(1-4) (2020).

* Joint research among groups within ISSP.

17. New phenomena of photo-luminescence and persistent luminescence of a Eu^{2+} ,Tb^{3+} codoped $Ca_6BaP_4O_{17}$ phosphor under high hydrostatic pressure: H. Guo, T. Seto, T. Geng, B. Zou, G. Li, Y. Uwatoko, Z. Tang, Z. Li and Y. Wang, Dalton Trans. **49**, 8056-2059 (2020).

18. Resistive anisotropy of candidate excitonic insulator Ta_2NiSe_5 under pressure: H. Arima, Y. Naito, K. Kudo, N. Katayama, H. Sawa, M. Nohara, Y. F. Lu, K. Kitagawa, H. Takagi, Y. Uwatoko and K. Matsubayashi, J. Phys.: Conf. Ser. **1609**, 012001(1-6) (2020).

19. Pressure-Driven Eu^{2+}-Doped $BaLi_2Al_2Si_2N_6$: A New Color Tunable Narrow-Band Emission Phosphor for Spectroscopy and Pressure Sensor Applications: Y. Wang, T. Seto, K. Ishigaki, Y. Uwatoko, G. Xiao, B. Zou, G. Li, Z. Tang, Z. Li and Y. Wang, Adv. Funct. Mater. **1**, 2001384(1-10) (2020).

20. *Single Crystal Growth and Unique Electronic States of Cubic Chiral EuPtSi and Related Compounds: Y. Ônuki, M. Kakihana, W. Iha, K. Nakaima, D. Aoki, A. Nakamura, F. Honda, M. Nakashima, Y. Amako, J. Gouchi, Y. Uwatoko, S. Nakamura, T. Sakakibara, T. Takeuchi, Y. Haga, H. Ikeda, H. Harima, M. Hedo and T. Nakama, JPS Conf. Proc. **29**, 012001(1-9) (2020).

21. *Unique Skyrmion Phases and Conduction Electrons in Cubic Chiral Antiferromagnet EuPtSi and Related Compounds: Y. Ônuki, M. Kakihana, W. Iha, K. Nakaima, D. Aoki, A. Nakamura, F. Honda, M. Nakashima, Y. Amako, J. Gouchi, Y. Uwatoko, S. Nakamura, T. Sakakibara, T. Takeuchi, Y. Haga, H. Ikeda, H. Harima, M. Hedo and T. Nakama, JPS Conf. Proc. **30**, 011008(1-11) (2020).

22. Pressure-induced second high-T_c superconducting phase in the organic-ion-intercalated $(CTA)_{0.3}FeSe$ single crystal: J. P. Sun, M. Z. Shi, B. Lei, S. X. Xu, Y. Uwatoko, X. H. Chen and J. -G. Cheng, EPL **130**, 67004(1-5) (2020).

23. Pressure effect on the anomalous Hall effect of ferromagnetic Weyl semimetal $Co_3Sn_2S_2$: Z. Y. Liu, T. Zhang, S. X. Xu, P. T. Yang, Q. Wang, H. C. Lei, Y. Sui, Y. Uwatoko, B. S. Wang, H. M. Weng, J. P. Sun and J. -G. Cheng, Phys. Rev. Materials **4**, 044203(1-9) (2020).

24. Fabrication and evaluation via nuclear quadrupole resonance of a palm cubic-anvil pressure cell: S. Nakagawa, J. Gochi, T. Kuwayama, S. Nagasaki, T. Takahashi, J. Cheng, Y. Uwatoko and N. Fujiwara, Review of Scientific Instruments **91**, 073907(1-7) (2020).

25. Heat treatment effect on the magnetic properties and martensitic transformations of MnCoGe: K. Noguchi, R. Kobayashi, Y. Mitsui, R. Y. Umetsu, J. Gouchi, Y. Uwatoko and K. Koyama, Journal of Magnetism and Magnetic Materials **499**, 166199(1-5) (2020).

26. Magnetic field-induced nitridation of Sm_2Fe_{17}: M. Onoue, R. Kobayashi, Y. Mitsui, R. Y. Umetsu, Y. Uwatoko and K. Koyama, Journal of Alloys and Compounds **835**, 155193(1-7) (2020).

27. Superconducting-Gap Anisotropy of Iron Pnictides Investigated via Combinatorial Microwave Measurements: T. Okada, Y. Imai, K. Kitagawa, K. Matsubayashi, M. Nakajima, A. Iyo, Y. Uwatoko, H. Eisaki and A. Maeda, Sci Rep **10**, 7064(1-7) (2020).

28. Quasi-one-dimensional magnetic interactions and conduction electrons in $EuCu_5$ and $EuAu_5$ with the characteristic hexagonal structure: S. Matsuda, J. Ota, K. Nakaima, W. Iha, J. Gouchi, Y. Uwatoko, M. Nakashima, Y. Amako, F. Honda, D. Aoki, A. Nakamura, T. Takeuchi, Y. Haga, H. Harima, M. Hedo, T. Nakama and Y. Ônuki, Philosophical Magazine **JAN 2020**, 1-14 (2020).

29. Redetermination of the crystal structure of R_5Si_4(R= Pr, Nd) from single-crystal X-ray diffraction data: K. Yokota, R. Watanuki, M. Nakashima, M. Uehara, J. Gouchi, Y. Uwatoko and I. Umehara, Acta Crystallogr E Cryst Commun **76**, 510 (2020).

30. Pressure-Induced Metallization and Structural Phase Transition in the Quasi-One-Dimensional $TlFeSe_2$: Z.-Y. Liu, Q.-X. Dong, P.-F. Shan, Y.-Y. Wang, J.-H. Dai, R. Jana, K.-Y. Chen, J.-P. Sun, B.-S. Wang, X.-H. Yu, G.-T. Liu, Y. Uwatoko, Y. Sui, H.-X. Yang, G.-F. Chen and J.-G. Cheng, Chinese Phys. Lett. **37**, 047102 (2020).

31. Crystallographic and superconducting properties of filled skutterudite $SrOs_4P_{12}$: Y. Kawamura, S. Deminami, K. Takeda, T. Kuzuya, L. Salamakha, H. Michor, E. Bauer, J. Gouchi, Y. Uwatoko, T. Kawae and C. Sekine, Phys. Rev. B **103**, 085139(1-9) (2021).

32. *Strongly correlated superconductivity in a copper-based metal-organic framework with a perfect kagome lattice: T. Takenaka, K. Ishihara, M. Roppongi, Y. Miao, Y. Mizukami, T. Makita, J. Tsurumi, S. Watanabe, J. Takeya, M. Yamashita, K. Torizuka, Y. Uwatoko, T. Sasaki, X. Huang, W. Xu, D. Zhu, N. Su, J. -G. Cheng, T. Shibauchi and K. Hashimoto, Sci. Adv. **7**, eabf3996(1-8) (2021).

33. Author Correction: Experimental evidence for the existence of a second partially-ordered phase of ice VI: R. Yamane,

† Joint research with outside partners.

K. Komatsu, J. Gouchi, Y. Uwatoko, S. Machida, T. Hattori, H. Ito and H. Kagi, Nat Commun **12**, 1800 (2021).

34. Experimental evidence for the existence of a second partially-ordered phase of ice VI: R. Yamane, K. Komatsu, J. Gouchi, Y. Uwatoko, S. Machida, T. Hattori, H. Ito and H. Kagi, Nat Commun **12**, 1129(1-6) (2021).

35. High-pressure phase diagrams of $FeSe_{1-x}Te_x$: correlation between suppressed nematicity and enhanced superconductivity: K. Mukasa, K. Matsuura, M. Qiu, M. Saito, Y. Sugimura, K. Ishida, M. Otani, Y. Onishi, Y. Mizukami, K. Hashimoto, J. Gouchi, R. Kumai, Y. Uwatoko and T. Shibauchi, Nat Commun **12**, 381(1-7) (2021).

36. Pressure induced superconducting state in ideal topological insulator $BiSbTe_3$: V. K. Gangwar, S. Kumar, M. Singh, L. Ghosh, Y. Zhang, P. Shahi, M. Muntwiler, S. Patil, K. Shimada, Y. Uwatoko, J. Sau, M. Kumar and S. Chatterjee, Phys. Scr. **96**, 055802(1-8) (2021).

37. Internal and External Pressure Effects on Superconductivity in $FeTe_xSe_{1-x}$ ($x = 0.46$, 0.54) Single Crystals: G. Lingannan, K. Ganesan, S. Mariappan, R. Sankar, Y. Uwatoko and S. Arumugam, J Supercond Nov Magn **34**, 725-731 (2021).

Ozaki group

In FY2020, we studied two issues: one is an investigation to unveil structural trends of ternary transition metal nano-particles, and the other is the first-principles calculation of superconducting transition temperature of elemental bulks. (1) As the first issue, we performed first-principles calculations and Monte Carlo sampling to investigate the structures of ternary PdRuM (M = Pt, Rh, or Ir) nanoparticles (NPs) with respect to three different spherical shapes. The calculations show that the atomic position is dominant in determining the stability of the ternary NPs. For bare ternary NPs, Pd and Ru atoms favor a location on the vertex sites and the core, respectively, which can be understood by the surface energy of the corresponding slab models. For single-crystalline NPs, the binary shell could be either a solid solution or a segregation alloy depending on composition and morphology. However, polycrystalline Ih NPs only form segregated binary shells surrounding the Ru core. Such configurations tend to minimize the surface lattice to gain more energy from the d orbital of the transition metals. In addition to the bare NPs, we study the oxidized ternary NPs. The results show that the Ru atoms penetrate outwards from the core to the surface reducing the oxidation formation energy. This work clearly demonstrates the structural trends of small ternary NPs, unveiling that the structural trends can be understood by the surface formation energy and the interplay between adsorbent and adsorbing oxygen atoms. (2) As the second issue, we performed systematic calculations to understand the applicability and limitation of Density functional theory for superconductors (SCDFT), which is one of the first-principles methods to compute Tc, and can treat the electron-phonon interaction, electronic Coulomb interaction, and spin fluctuation (SF) fully non-empirically. This method has been applied to mainly the phonon-mediated superconductors. For example, SCDFT is used to reveal the origin of the multi-band superconductivity in MgB, the relationship between the structure and Tc of hydrogen sulfides. We plan to apply this method to a wide variety of materials and accelerate the first-principles exploration of superconductors. For this purpose, we are developing an open-source software Superconducting-Toolkit (SCTK), and release that software on the Web. In this study, we performed a benchmark to the simplest superconductors and non-superconductors, namely 35 elemental metals; we formulated a method to treat SF together with the spin-orbit interaction (SOI) and investigate these two effects on Tc. We believe that this benchmark study will be a milestone for exploring superconductors with high-throughput computations and methodological improvements in the future.

1. Benchmark of density functional theory for superconductors in elemental materials: M. Kawamura, Y. Hizume and T. Ozaki, Phys. Rev. B **101**, 134511 (2020).

2. *Emergence of nearly flat bands through a kagome lattice embedded in an epitaxial two-dimensional Ge layer with a bitriangular structure: A. Fleurence, C. -C. Lee, R. Friedlein, Y. Fukaya, S. Yoshimoto, K. Mukai, H. Yamane, N. Kosugi, J. Yoshinobu, T. Ozaki and Y. Yamada-Takamura, Phys. Rev. B **102**, 201102 (2020).

3. First-principles study on the stability and electronic structure of monolayer GaSe with trigonal-antiprismatic structure: H. Nitta, T. Yonezawa, A. Fleurence, Y. Yamada-Takamura and T. Ozaki, Phys. Rev. B **102**, 235407 (2020).

4. Unfolding optical transition weights of impurity materials for first-principles LCAO electronic structure calculations: Y.-T. Lee, C.-C. Lee, M. Fukuda and T. Ozaki, Phys. Rev. B **102**, 075143 (2020).

5. *Formation of BN-covered silicene on ZrB_2/Si(111) by adsorption of NO and thermal processes: J. Yoshinobu, K. Mukai, H. Ueda, S. Yoshimoto, S. Shimizu, T. Koitaya, H. Noritake, C.-C. Lee, T. Ozaki, A. Fleurence, R. Friedlein and Y. Yamada-Takamura, J. Chem. Phys. **153**, 064702 (2020).

6. *Structural investigation of ternary PdRuM (M = Pt, Rh, or Ir) nanoparticles using first-principles calculations: S.-H. Hung, H. Akiba, O. Yamamuro and T. Ozaki, RSC Adv. **10**, 16527 (2020).

7. *Electronic structure of a (3×3)-ordered silicon layer on Al(111): Y. Sato, Y. Fukaya, M. Cameau, A. K. Kundu, D. Shiga, R. Yukawa, K. Horiba, C.-H. Chen, A. Huang, H.-T. Jeng, T. Ozaki, H. Kumigashira, M. Niibe and I.

* Joint research among groups within ISSP.

Matsuda, Phys. Rev. Materials **4**, 064005 (2020).

8. Neural network atomic potential to investigate the dislocation dynamics in bcc iron: H. Mori and T. Ozaki, Phys. Rev. Materials **4**, 040601(R) (2020).

9. *Vapochromism induced by intermolecular electron transfer coupled with hydrogen-bond formation in zinc dithiolene complex: T. Fujino, M. Kawamura, T. Ozaki and H. Mori, J. Mater. Chem. C **8**, 14939-14947 (2020).

10. First-principles adaptive-boost accelerated molecular dynamics simulation with effective boost potential construction methods: a study of Li diffusion in Si crystal: M. Yamamoto, A. Ishii, S. Shinzato, S. Ogata and T. Ozaki, Japanese Journal of Applied Physics **59**, 125002 (2020).

11. Diverse densest binary sphere packings and phase diagram: R. Koshoji, M. Kawamura, M. Fukuda and T. Ozaki, Phys. Rev. E **103**, 023307 (2021).

12. †*Kω— Open-source library for the shifted Krylov subspace method of the form $(zI - H)x = b$: T. Hoshi, M. Kawamura, K. Yoshimi, Y. Motoyama, T. Misawa, Y. Yamaji, S. Todo, N. Kawashima and T. Sogabe, Computer Physics Communications **258**, 107536 (2021).

13. †*RESPACK: An ab initio tool for derivation of effective low-energy model of material: K. Nakamura, Y. Yoshimoto, Y. Nomura, T. Tadano, M. Kawamura, T. Kosugi, K. Yoshimi, T. Misawa and Y. Motoyama, Computer Physics Communications **261**, 107781 (2021).

14. Structure of one-dimensional monolayer Si nanoribbons on Ag(111): L. Feng, A. Shiotari, K. Yabuoshi, M. Fukuda, T. Ozaki and Y. Sugimoto, Phys. Rev. Materials **5**, 034002 (2021).

15. *The Simplest Model for Doped Poly(3,4-ethylenedioxythiophene) (PEDOT): Single-crystalline EDOT Dimer Radical Cation Salts: R. Kameyama, T. Fujino, S. Dekura, M. Kawamura, T. Ozaki and H. Mori, Chem. Eur. J. **27**, 6696 (2021).

Noguchi group

We have studied (1) Turing patterns on a vesicle by a reaction-diffusion system coupled with mechanochemical feedback, (2) the conformation of ultra-long-chain fatty acid in lipid bilayer, (3) the effects of cavitation on Karman vortex, and (4) sound-wave propagation in a simple fluid. We also proposed (5) a new numerical method to calculate membrane mechanical properties.

1. †Conformation of ultra-long-chain fatty acid in lipid bilayer: Molecular dynamics study: K. Kawaguchi, K. M. Nakagawa, S. Nakagawa, H. Shindou, H. Nagao and H. Noguchi, J. Chem. Phys. **153**, 165101 (2020).

2. †Effects of cavitation on Kármán vortex behind circular-cylinder arrays: A molecular dynamics study: Y. Asano, H. Watanabe and H. Noguchi, J. Chem. Phys. **152**, 034501 (2020).

3. †Molecular dynamics simulation of soundwave propagation in a simple fluid: Y. Asano, H. Watanabe and H. Noguchi, J. Chem. Phys. **153**, 124504 (2020).

4. †Virtual bending method to calculate bending rigidity, saddle-splay modulus, and spontaneous curvature of thin fluid membranes: H. Noguchi, Phys. Rev. E **102**, 053315 (2020).

5. Supramolecular Biocomposite Hydrogels Formed by Cellulose and Host–Guest Polymers Assisted by Calcium Ion Complexes: H. Tsuchiya, G. Sinawang, T.-A. Asoh, M. Osaki, Y. Ikemoto, Y. Higuchi, H. Yamaguchi, A. Harada, H. Uyama and Y. Takashima, Biomacromolecules **21**, 3936 (2020).

6. Pattern formation in reaction–diffusion system on membrane with mechanochemical feedback: N. Tamemoto and H. Noguchi, Sci Rep **10**, 19582 (2020).

7. * 分子動力学計算による複雑流体中のカルマン渦の解析 : 浅野 優太 , 渡辺 宙志 , 野口 博司 , 分子シミュレーション学会誌 " アンサンブル " **22**, 157-162 (2020).

8. †Rational Design Principles of Attenuated Cationic Lytic Peptides for Intracellular Delivery of Biomacromolecules: N. Tamemoto, M. Akishiba, K. Sakamoto, K. Kawano, H. Noguchi and S. Futaki, Mol. Pharmaceutics **17**, 2175-2185 (2020).

9. 高分子材料の破壊に関する粗視化シミュレーション : 樋口 祐次 , 分子シミュレーション学会誌「アンサンブル」**22**, 216-221 (2020).

10. Coarse-grained molecular dynamics simulations of void generation and growth processes in the fracture of the lamellar structure of polyethylene: Y. Higuchi, Phys. Rev. E **103**, 042502 (2021).

† Joint research with outside partners.

11. Undulation of a moving fluid membrane pushed by filament growth: H. Noguchi and O. Pierre-Louis, Sci Rep **11**, 7985 (2021).

Yoshimi group

We have developed and enhanced the usability of programs adopted in the project for advancement of software usability in materials science (PASUMS). Our group's activity of 2020 include development of (1) optimization tools for PHYSics based on Bayesian Optimization (PHYSBO), (2) 2DMAT, and the enhancement of usability for (3) MateriApps Installer. In addition, we have studied (1) derivation and analysis of low-energy effective Hamiltonian of organic conductors using software packages (RESPACK and HΦ) developed in PASUMS and (2) application of sparse modeling in quantum many body problems.

1. †Finite Temperature Properties of Geometrically Charge Frustrated Systems: K. Yoshimi, M. Naka and H. Seo, J. Phys. Soc. Jpn. **89**, 034003 (2020).

2. †Sparse Modeling in Quantum Many-Body Problems: J. Otsuki, M. Ohzeki, H. Shinaoka and K. Yoshimi, J. Phys. Soc. Jpn. **89**, 012001 (2020).

3. †Transport properties of the organic Dirac electron system α-$(BEDT-TSeF)_2I_3$: D. Ohki, K. Yoshimi and A. Kobayashi, Phys. Rev. B **102**, 235116 (2020).

4. †Electronic correlation and geometrical frustration in molecular solids: A systematic ab initio study of β'$-X[Pd(dmit)_2]_2$: T. Misawa, K. Yoshimi and T. Tsumuraya, Phys. Rev. Research **2**, 032072 (2020).

5. †Sparse sampling and tensor network representation of two-particle Green's functions: H. Shinaoka, D. Geffroy, M. Wallerberger, J. Otsuki, K. Yoshimi, E. Gull and J. Kuneš, SciPost Phys. **8**, 012 (2020).

6. †Multiple-magnon excitations shape the spin spectrum of cuprate parent compounds: D. Betto, R. Fumagalli, L. Martinelli, M. Rossi, R. Piombo, K. Yoshimi, D. D. Castro, E. D. Gennaro, A. Sambri, D. Bonn, G. A. Sawatzky, L. Braicovich, N. B. Brookes, J. Lorenzana and G. Ghiringhelli, Phys. Rev. B **103**, L140409 (2021).

7. †*DSQSS: Discrete Space Quantum Systems Solver: Y. Motoyama, K. Yoshimi, A. Masaki-Kato, T. Kato and N. Kawashima, Computer Physics Communications **264**, 107944 (2021).

8. †*Kω— Open-source library for the shifted Krylov subspace method of the form $(zI - H)x = b$: T. Hoshi, M. Kawamura, K. Yoshimi, Y. Motoyama, T. Misawa, Y. Yamaji, S. Todo, N. Kawashima and T. Sogabe, Computer Physics Communications **258**, 107536 (2021).

9. †*RESPACK: An ab initio tool for derivation of effective low-energy model of material: K. Nakamura, Y. Yoshimoto, Y. Nomura, T. Tadano, M. Kawamura, T. Kosugi, K. Yoshimi, T. Misawa and Y. Motoyama, Computer Physics Communications **261**, 107781 (2021).

Materials Synthesis and Characterization group

1. Anisotropic Magnetic Field Dependence of Specific Heat in the Cubic Symmetric Quadrupolar Kondo Compound $Pr_{0.05}La_{0.95}Pb_3$: T. Kawae, M. Koga, Y. Sato, Y. Inagaki, T. Fujiwara, H. S. Suzuki and T. Kitai, J. Phys. Soc. Jpn. **89**, 063704 (2020).

2. Kondo-Induced Giant Isotropic Negative Thermal Expansion: D. G. Mazzone, M. Dzero, AM. M. Abeykoon, H. Yamaoka, H. Ishii, N. Hiraoka, J. -P. Rueff, J. M. Ablett, K. Imura, H. S. Suzuki, J. N. Hancock and I. Jarrige, Phys. Rev. Lett. **124**, 125701 (2020).

3. *Anisotropic Triangular Lattice Realized in Rhenium Oxychlorides $A_3ReO_5Cl_2$ (A = Ba, Sr): D. Hirai, T. Yajima, K. Nawa, M. Kawamura and Z. Hiroi, Inorg. Chem. **59**, 10025 (2020).

4. *Spin–orbit-coupled metal candidate $PbRe_2O_6$: S. Tajima, D. Hirai, T. Yajima, D. Nishio-Hamane, Y. Matsubayashi and Z. Hiroi, Journal of Solid State Chemistry **288**, 121359 (2020).

5. Magnetic properties of oxides with high concentrations of rare-earth elements R_6AO_{12} (R = rare-earth element, A = Mo or W): M. Hase, N. Tsujii, H. S. Suzuki, O. Sakai and H. Mamiya, Journal of Magnetism and Magnetic Materials **523**, 167539 (2020).

6. *Devil's staircase transition of the electronic structures in CeSb: K. Kuroda, Y. Arai, N. Rezaei, S. Kunisada, S. Sakuragi, M. Alaei, Y. Kinoshita, C. Bareille, R. Noguchi, M. Nakayama, S. Akebi, M. Sakano, K. Kawaguchi, M. Arita, S. Ideta, K. Tanaka, H. Kitazawa, K. Okazaki, M. Tokunaga, Y. Haga, S. Shin, H. S. Suzuki, R. Arita and T. Kondo, Nat Commun **11**, 2888/1-9 (2020).

* Joint research among groups within ISSP.

Neutron Science Laboratory

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. The highlight of this year is the inelastic neutron scattering (INS) experiment of vapor-deposited CS_2 glass which was performed on AMATERAS in J-PARC MLF. By combining the results of CS_2 and CCl_4, which was measured in 2018, we have found the general relation between the low-energy excitations and local structures in the glass. The boson peak appears independently of the local structure of the glass, while the dispersive phonon excitations adjacent to the boson peak strongly depends on the quasi-network structure of the glass. Following the quasi-elastic neutron scattering (QENS) of a novel hydrogen-cluster material Li_6NbH_{11} measured last year, the QENS experiment of Li_5MoH_{11} was carried out on DNA in J-PARC MLF. Both data demonstrate that the MH_9 cluster is rotating rapidly with widely-distributed relaxation times, which may be caused by the conducting (positionally disordered) Li ions. The correlation between the conducting Li ions and hydrogen clusters was found also in the calorimetric experiment of novel Li conductors containing cage-like ions, $Li(CB_9H_{10})$ and $0.7Li(CB_9H_{10})$-$0.3Li(CB_{11}H_{12})$. The synchrotron-radiation X-ray diffraction experiment was conducted in SPring-8 for the glass of a novel metal-organic framework (MOF) material containing CO_2 as guest molecules.

1. Dynamics of Atomic Hydrogen in Palladium Probed by Neutron Spectroscopy: M. Kofu and O. Yamamuro, J. Phys. Soc. Jpn. **89**, 051002 (2020).

2. Rational Synthesis for a Noble Metal Carbide: T. Wakisaka, K. Kusada, D. Wu, T. Yamamoto, T. Toriyama, S. Matsumura, H. Akiba, O. Yamamuro, K. Ikeda, T. Otomo, N. Palina, Y. Chen, L. S. R. Kumara, C. Song, O. Sakata, W. Xie, M. Koyama, Y. Kubota, S. Kawaguchi, R. L. Arevalo, S. M. Aspera, E. F. Arguelles, H. Nakanishi and H. Kitagawa, J. Am. Chem. Soc. **142**, 1247 (2020).

3. New Insights on the Formation Process and Thermodynamics of the α-Phase $PdH(D)_x$ through Direct Enthalpy Measurement of H(D) Dissolution: S. Dekura, H. Akiba, O. Yamamuro, H. Kobayashi, M. Maesato and H. Kitagawa, J. Phys. Chem. C **124**, 8663-8668 (2020).

4. Nanometric Fluctuations of Sound Velocity in Alkali Borate Glasses and Fragility of Respective Melts: S. Kojima, V. N. Novikov, M. Kofu and O. Yamamuro, Phys. Status Solidi B **257**, 2000073 (2020).

5. Nanoscale Relaxation in "Water-in-Salt" and "Water-in-Bisalt" Electrolytes: M. A. González, O. Borodin, M. Kofu, K. Shibata, T. Yamada, O. Yamamuro, K. Xu, D. L. Price and M. -L. Saboungi, J. Phys. Chem. Lett. **11**, 7279 (2020).

6. [*]Structural investigation of ternary PdRuM (M = Pt, Rh, or Ir) nanoparticles using first-principles calculations: S.-H. Hung, H. Akiba, O. Yamamuro and T. Ozaki, RSC Adv. **10**, 16527 (2020).

7. Quasielastic Neutron Scattering Study on Polymorphism of Glycerol Deuterated Triacylglycerols: Comparison with Saturated, Trans-unsaturated and Cis-unsaturated Triacylglycerols: C. Takechi, T. Kawaguchi, F. Kaneko and O. Yamamuro, Chem. Lett. **50**, 435 (2021).

8. ガラス転移温度 : 山室 修 ,「化学便覧基礎編改訂第 6 版」, 10.15, 日本化学会編 , (丸善出版 , 2020), 77-81.

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; Helical and collinear spin density wave order in the S = 1/2 one-dimensional frustrated chain compound $NaCuMoO_4(OH)$ investigated by neutron scattering, Magnetic order in the chemically substituted frustrated antiferromagnet $CsCrF_4$, Zero-energy excitation in the classical kagome antiferromagnet $NaBa_2Mn_3F_{11}$, Magnetic correlations in $YBaCo_4O_7$ on kagome and triangular lattices, etc.

1. Analysis of Field-Induced Nonreciprocal Magnon in Noncollinear Magnet and Application to S = 1 Triangular Antiferromagnet $CsFeCl_3$: M. Matsumoto, S. Hayashida and T. Masuda, J. Phys. Soc. Jpn. **89**, 034710(1-17) (2020).

2. Horizontal Line Nodes in Sr_2RuO_4 Proved by Spin Resonance: K. Iida, M. Kofu, K. Suzuki, N. Murai, S. Ohira-Kawamura, R. Kajimoto, Y. Inamura, M. Ishikado, S. Hasegawa, T. Masuda, Y. Yoshida, K. Kakurai, K. Machida and S. Lee, J. Phys. Soc. Jpn. **89**, 053702(1-5) (2020).

3. Mossbauer Study of Rare-earth Ferroborate $NdFe_3(BO_3)_4$: S. Nakamura, T. Masuda, K. Ohgushi and T. Katsufuji, J. Phys. Soc. Jpn. **89**, 084703(1-6) (2020).

4. [†*]Emergent spin-1 Haldane gap and ferroelectricity in a frustrated spin- 1/2 ladder: H. Ueda, S. Onoda, Y. Yamaguchi, T. Kimura, D. Yoshizawa, T. Morioka, M. Hagiwara, M. Hagihala, M. Soda, T. Masuda, T. Sakakibara, K. Tomiyasu,

[†] Joint research with outside partners.

S. Ohira-Kawamura, K. Nakajima, R. Kajimoto, M. Nakamura, Y. Inamura, N. Reynolds, M. Frontzek, J. S. White, M. Hase and Y. Yasui, Phys. Rev. B **101**, 140408(1-6) (2020).

5. *Helical and collinear spin density wave order in the S = 1/2 one-dimensional frustrated chain compound $NaCuMoO_4(OH)$ investigated by neutron scattering: S. Asai, T. Oyama, K. Nawa, A. Nakao, K. Munakata, K. Kuwahara, M. Hagihala, S. Itoh, Z. Hiroi and T. Masuda, Phys. Rev. B **101**, 144437(1-8) (2020).

6. Magnetic correlations in $YBaCo_4O_7$ on kagome and triangular lattices: M. Soda, S. Itoh, T. Yokoo, G. Ehlers, H. Kawano-Furukawa and T. Masuda, Phys. Rev. B **101**, 214444(1-7) (2020).

7. Magnetic order in the chemically substituted frustrated antiferromagnet $CsCrF_4$: S. Hayashida, M. Hagihala, M. Avdeev, Y. Miura, H. Manaka and T. Masuda, Phys. Rev. B **102**, 174440(1-6) (2020).

8. Spin waves in the two-dimensional honeycomb lattice XXZ-type van der Waals antiferromagnet CoPS3: C. Kim, J. Jeong, P. Park, T. Masuda, S. Asai, S. Itoh, H.-S. Kim, A. Wildes and J.-G. Park, Phys. Rev. B **102**, 184429(1-8) (2020).

9. *Zero-energy excitation in the classical kagome antiferromagnet $NaBa_2Mn_3F_{11}$: S. Hayashida, H. Ishikawa, Y. Okamoto, T. Okubo, Z. Hiroi, G. J. Nilsen, H. Mutka and T. Masuda, Phys. Rev. B **101**, 214409 (2020).

10. The f-electron State of the Heavy Fermion Superconductor $NpPd_5Al_2$ and the Isostructural Family: N. Metoki, A. A. Aczel, D. Aoki, S. Chi, J. A. Fernandez-Baca, J.-C. Griveau, M. Hagihala, T. Hong, Y. Haga, K. Ikeuchi, Y. Inamura, K. Kamazawa, R. Kajimoto, H. Kitazawa, T. Masuda, M. Matsuda, M. Nakamura, J. Ohtsuki, D. Pajerowski, H. S. Suzuki, E. Yamamoto and H. Yamauchi, JPS Conf. Proc. **30**, 011123(1-6) (2020).

11. Establishing the carrier scattering phase diagram for ZrNiSn-based half-Heusler thermoelectric materials: Q. Ren, C. Fu, Q. Qiu, S. Dai, Z. Liu, T. Masuda, S. Asai, M. Hagihala, S. Lee, S. Torri, T. Kamiyama, L. He, X. Tong, C. Felser, D. J. Singh, T. Zhu, J. Yang and J. Ma, Nat Commun **11**, 3142(1-9) (2020).

12. †*Gapless spin liquid in a square-kagome lattice antiferromagnet: M. Fujihala, K. Morita, R. Mole, S. Mitsuda, T. Tohyama, S.-I. Yano, D. Yu, S. Sota, T. Kuwai, A. Koda, H. Okabe, H. Lee, S. Itoh, T. Hawai, T. Masuda, H. Sagayama, A. Matsuo, K. Kindo, S. Ohira-Kawamura and K. Nakajima, Nat Commun **11**, 3429 (2020).

13. Fermionic order by disorder in a van der Waals antiferromagnet: R. Okuma, D. Ueta, S. Kuniyoshi, Y. Fujisawa, B. Smith, C. H. Hsu, Y. Inagaki, W. Si, T. Kawae, H. Lin, F. C. Chuang, T. Masuda, R. Kobayashi and Y. Okada, Sci Rep **10**, 15311(8pages) (2020).

14. Dynamical Studies in Condensed Matter on High Resolution Chopper Spectrometer (HRC) —2nd Phase of HRC Project—: S. Itoh, T. Masuda, T. Yokoo, H. Yoshizawa, M. Soda, S. Asai, Y. Ikeda, S. Ibuka, M. Yoshida, T. Hawai, H. Saito, D. Kawana, R. Sugiura, T. Asami and Y. Ihata, JPS Conf. Proc. **33**, 011058(1-7) (2021).

Nakajima group

Nakajima group has been studying magnetic materials showing cross-correlated phenomena related to topologically-nontrivial magnetic structures. One example is magnetic skyrmion, which is vortex-like spin order behaving like a particle. In this year, we investigated crystallization process of magnetic skyrmions in a chiral magnet MnSi by means of neutron resonance spin-echo spectroscopy in J-PARC. We have been collaborating with scientists in KEK and Kyoto university to develop the resonance-type neutron spin echo spectrometer, and successfully observed spin echo signals revealing that the spin fluctuations near the phase boundary between the paramagnetic and skyrmion lattice phases has a characteristic relaxation time of 1 ns. We also studied rare-earth based skyrmion materials by resonant X-ray magnetic scattering, and also applied polarized small-angle neutron scattering technique to a polar crystal hosting Neel-type magnetic skyrmion lattice.

1. 中性子散乱を用いた磁気スキルミオン研究 : 中島 多朗 , 有馬 孝尚 , 固体物理 **55**, 265-274 (2020).

2. Crystallization of magnetic skyrmions in MnSi investigated by neutron spin echo spectroscopy: T. Nakajima, T. Oda, M. Hino, H. Endo, K. Ohishi, K. Kakurai, A. Kikkawa, Y. Taguchi, Y. Tokura and T.-H. Arima, Phys. Rev. Research **2**, 043393 (2020).

3. Nanometric square skyrmion lattice in a centrosymmetric tetragonal magnet: N. D. Khanh, T. Nakajima, X. Yu, S. Gao, K. Shibata, M. Hirschberger, Y. Yamasaki, H. Sagayama, H. Nakao, L. Peng, K. Nakajima, R. Takagi, T.-H. Arima, Y. Tokura and S. Seki, Nat. Nanotechnol. **15**, 444 (2020).

4. Direct Observation of Cycloidal Spin Modulation and Field-induced Transition in Néel-type Skyrmion-hosting $VOSe_2O_5$: T. Kurumaji, T. Nakajima, A. Feoktystov, E. Babcock, Z. Salhi, V. Ukleev, T.-H. Arima, K. Kakurai and Y. Tokura, J. Phys. Soc. Jpn. **90**, 024705 (2021).

* Joint research among groups within ISSP.

Mayumi group

We have discovered that slide-ring gels, in which polymer chains are cross-linked by ring molecules, show strain-induced crystallization (SIC) under uniaxial stretching. The occurrence of SIC improves significantly the mechanical toughness of slide-ring gels. In addition, the crystalline formation is reversible in response to elongation and retraction, which results in the high mechanical reversibility under cyclic deformations. The novel toughening mechanism of hydrogels by SIC enables the simultaneous improvement of toughness and reversibility required for the applications of hydrogels as biomaterials, such as artificial cartilage and prosthetic joints.

International MegaGauss Science Laboratory

Kindo group

We have examined an Fulde–Ferrell–Larkin–Ovchinnikov phase using some angle-resolved physical property measurements in pulsed magnetic fields, which have unveiled details of pair-breaking effects of the magnetic field on this phase. Magnetism of the 4*d* and 5*d* transition metal double perovskites with strong spin-orbit coupling are investigated up to around 65 T. We discovered the ligand dependent magnetism in Cs_2MX_6 (M= Nb, Ta, X = Cl, Br) and the magnetic field induced phase transition at 50 T in Ba_2CaReO_6.

1. †Ga Substitution Effect on the Valence Transition of $Eu_2Pt_6Al_{15}$: K. Oyama, A. Mitsuda, H. Wada, Y. Narumi, M. Hagiwara, R. Takahashi, H. Wadati, H. Setoyama and K. Kindo, J. Phys. Soc. Jpn. **89**, 114713 (2020).

2. *Kitaev Spin Liquid Candidate Os_xCl_3 Comprised of Honeycomb Nano-Domains: K. Kataoka, D. Hirai, T. Yajima, D. Nishio-Hamane, R. Ishii, K.-Y. Choi, D. Wulferding, P. Lemmens, S. Kittaka, T. Sakakibara, H. Ishikawa, A. Matsuo, K. Kindo and Z. Hiroi, J. Phys. Soc. Jpn. **89**, 114709(1-9) (2020).

3. †Multi-Step Magnetic Transitions in $EuNiIn_4$: S. Ikeda, K. Kaneko, Y. Tanaka, T. Kawasaki, T. Hanashima, K. Munakata, A. Nakao, R. Kiyanagi, T. Ohhara, K. Mochizuki, A. Kondo, K. Kindo, Y. Homma, M. D. Frontzek and H. Kobayashi, J. Phys. Soc. Jpn. **89**, 014707(1-7) (2020).

4. †Vanishment of Metamagnetic Transition in the Metal-to-Insulator Transition Compound $BaVS_3$ under High Pressure: T. Tahara, T. Kida, Y. Narumi, T. Takeuchi, H. Nakamura, K. Miyake, K. Kindo and M. Hagiwara, J. Phys. Soc. Jpn. **89**, 064711(1-5) (2020).

5. †Angle-dependent nontrivial phase in the Weyl semimetal NbAs with anisotropic Fermi surface: M. Komada, H. Murakawa, M. S. Bahramy, T. Kida, K. Yokoi, Y. Narumi, K. Kindo, M. Hagiwara, H. Sakai and N. Hanasaki, Phys. Rev. B **101**, 045135(1-6) (2020).

6. †Data-driven determination of the spin Hamiltonian parameters and their uncertainties: The case of the zigzag-chain compound $KCu_4P_3O_{12}$: R. Tamura, K. Hukushima, A. Matsuo, K. Kindo and M. Hase, Phys. Rev. B **101**, 224435(1-9) (2020).

7. *Enhanced spin correlations in the Bose-Einstein condensate compound $Sr_3Cr_2O_8$: T. Nomura, Y. Skourski, D. L. Quintero-Castro, A. A. Zvyagin, A. V. Suslov, D. Gorbunov, S. Yasin, J. Wosnitza, K. Kindo, A. T. M. N. Islam, B. Lake, Y. Kohama, S. Zherlitsyn and M. Jaime, Phys. Rev. B **102**, 165144 (2020).

8. *Observation of in-plane magnetic field induced phase transitions in FeSe: J. M. Ok, C. I. Kwon, Y. Kohama, J. S. You, S. K. Park, J.-H. Kim, Y. J. Jo, E. S. Choi, K. Kindo, W. Kang, K.-S. Kim, E. G. Moon, A. Gurevich and J. S. Kim, Phys. Rev. B **101**, 224509 (2020).

9. *Quantum oscillations and magnetic field induced Fermi surface reconstruction in the charge density wave state of A0.9Mo6O17 (A = Na, K): H. P. Zhu, M. Yang, J. Z. Ke, H. K. Zuo, T. Peng, J. F. Wang, Y. Liu, X. Xu, Y. Kohama, K. Kindo and M. Greenblatt, Phys. Rev. B **102**, 235164 (2020).

10. Thermal and magnetoelastic properties of α−$RuCl_3$ in the field-induced low-temperature states: R. Schönemann, S. Imajo, F. Weickert, J. Yan, D. G. Mandrus, Y. Takano, E. L. Brosha, P. F. S. Rosa, S. E. Nagler, K. Kindo and M. Jaime, Phys. Rev. B **102**, 214432(1-7) (2020).

11. *Anisotropic Fully Gapped Superconductivity Possibly Mediated by Charge Fluctuations in a Nondimeric Organic Complex: S. Imajo, H. Akutsu, R. Kurihara, T. Yajima, Y. Kohama, M. Tokunaga, K. Kindo and Y. Nakazawa, Phys. Rev. Lett. **125**, 177002 (2020).

12. †Nonmagnetic Ground States and a Possible Quadrupolar Phase in 4*d* and 5*d* Lacunar Spinel Selenides GaM_4Se_8 (M =

† Joint research with outside partners.

Nb, Ta): H. Ishikawa, T. Yajima, A. Matsuo, Y. Ihara and K. Kindo, Phys. Rev. Lett. **124**, 227202(1-6) (2020).

13. †*Particle-Hole Symmetry Breaking in a Spin-Dimer System $TlCuCl_3$ Observed at 100 T: X. -G. Zhou, Y. Yao, Y. H. Matsuda, A. Ikeda, A. Matsuo, K. Kindo and H. Tanaka, Phys. Rev. Lett. **125**, 267207 1-6 (2020).
14. †*Synthesis, Structure, and Anomalous Magnetic Ordering of the Spin-1/2 Coupled Square Tetramer System K(NbO) $Cu_4(PO_4)_4$: K. Kimura, D. Urushihara, T. Asaka, M. Toyoda, A. Miyake, M. Tokunaga, A. Matsuo, K. Kindo, K. Yamauchi and T. Kimura, Inorg. Chem. **59**, 10986-10995 (2020).
15. *Extracting the Chiral Contribution to the Negative Longitudinal Magnetoresistance in Epitaxial $Pr_2Ir_2O_7$ Thin Films: T. Ohtsuki, Z. Tian, A. Endo, M. Halim, S. Katsumoto, Y. Kohama, K. Kindo, M. Lippmaa and S. Nakatsuji, JPS Conf. Proc. **30**, 011181 (1-6) (2020).
16. Avoided quantum criticality and cluster-glass formation in itinerant ferromagnet $Sr_{1-x}(La_{0.5}K_{0.5})_xRuO_3$: R. Iwahara, R. Sugawara, *. Rahmanto, Y. Honma, K. Matsuoka, A. Matsuo, K. Kindo, K. Tenya and M. Yokoyama, Phys. Rev. Materials **4**, 074404(1-8) (2020).
17. *Improved accuracy in high-frequency AC transport measurements in pulsed high magnetic fields: H. Mitamura, R. Watanuki, E. Kampert, T. Förster, A. Matsuo, T. Onimaru, N. Onozaki, Y. Amou, K. Wakiya, K. T. Matsumoto, I. Yamamoto, K. Suzuki, S. Zherlitsyn, J. Wosnitza, M. Tokunaga, K. Kindo and T. Sakakibara, Review of Scientific Instruments **91**, 125107/1-25 (2020).
18. †*Gapless spin liquid in a square-kagome lattice antiferromagnet: M. Fujihala, K. Morita, R. Mole, S. Mitsuda, T. Tohyama, S.-I. Yano, D. Yu, S. Sota, T. Kuwai, A. Koda, H. Okabe, H. Lee, S. Itoh, T. Hawai, T. Masuda, H. Sagayama, A. Matsuo, K. Kindo, S. Ohira-Kawamura and K. Nakajima, Nat Commun **11**, 3429 (2020).
19. *High-field phase diagram of $Ni_3V_2O_8$ studied by specific heat and magnetocaloric effect measurements: C. Dong, Y. Kohama, Z. Z. He, X. T. Han, K. Sato, A. Matsuo, K. Kindo, M. Yang and J. F. Wang, J. Phys.: Condens. Matter **33**, 205402 (2021).
20. Ligand dependent magnetism of the $J = 3/2$ Mott insulator Cs_2MX_6 (M = Ta, Nb, X = Br, Cl): H. Ishikawa, T. Yajima, A. Matsuo and K. Kindo, J. Phys.: Condens. Matter **33**, 125802(1-6) (2021).
21. Magnetization Process in $EuCo_2P_2$ and EuT_2Ge_2 (T: transition metal): Comparison of Experiment and Theory: T. Takeuchi, T. Tahara, T. Kida, Y. Narumi, M. Hagiwara, K. Kindo, W. Iha, Y. Ashitomi, T. Yara, M. Nakashima, Y. Amako, M. Hedo, T. Nakama and Y. Onuki, J. Phys. Soc. Jpn. **90**, 034709(1-15) (2021).
22. †*Spin Excitations of the $S = 1/2$ One-Dimensional Ising-Like Antiferromagnet $BaCo_2V_2O_8$ in Transverse Magnetic Fields: A. Okutani, H. Onishi, S. Kimura, T. Takeuchi, T. Kida, M. Mori, A. Miyake, M. Tokunaga, K. Kindo and M. Hagiwara, J. Phys. Soc. Jpn. **90**, 044704/1-9 (2021).
23. †*Geometrical Hall effect and momentum-space Berry curvature from spin-reversed band pairs: M. Hirschberger, Y. Nomura, H. Mitamura, A. Miyake, T. Koretsune, Y. Kaneko, L. Spitz, Y. Taguchi, A. Matsuo, K. Kindo, R. Arita, M. Tokunaga and Y. Tokura, Phys. Rev. B **103**, L041111(1-6) (2021).
24. Symmetry change of d-wave superconductivity in κ-type organic superconductors: S. Imajo, K. Kindo and Y. Nakazawa, Phys. Rev. B **103**, L060508(1-5) (2021).
25. *Compact megajoule-class pulsed power supply for generating long-pulsed magnetic fields: K. Matsui, T. Kanda, Y. Ihara, K. Kindo and Y. Kohama, Review of Scientific Instruments **92**, 024711 (2021).
26. *High-resolution calorimetry in pulsed magnetic fields: S. Imajo, C. Dong, A. Matsuo, K. Kindo and Y. Kohama, Review of Scientific Instruments **92**, 043901 (2021).

Tokunaga group

In this year, we have developed or improved several measurements in high magnetic fields. Using fast capacitance measurements, we have achieved high-precision measurements of magnetostriction, dielectric constants, and magnetocaloric effects in pulsed-high magnetic fields. We utilize polarizing microscopy to visualize domain structures in CeSb and $Cd_2Re_2O_7$ and study the dynamics of superconducting vortices and field-induced structural transitions in metamagnetic shape memory alloys using a high-speed camera. Utilizing various measurement techniques, we studied magnetic field-induced phase transitions in several heavy fermion and multiferroic materials and magnetotransport properties of topological semimetals. In elemental tellurium, a semiconductor with a chiral crystal structure, our high-field magnetotransport study revealed the existence of metallic states on the as-cleavage surfaces of single crystals.

1. *^{105}Pd NMR and NQR study of the cubic heavy fermion system $Ce_3Pd_{20}Si_6$: I. Jakovac, M. Horvatic, E. F. Schwier,

* Joint research among groups within ISSP.

A. Prokofiev, S. Paschen, H. Mitamura, T. Sakakibara and M. S. Grbic, J. Phys.: Condens. Matter **32**, 245601(1-7) (2020).

2. *Domain Control by Adjusting Anisotropic Stress in Pyrochlore Oxide $Cd_2Re_2O_7$: S. Tajima, D. Hirai, Y. Kinoshita, M. Tokunaga, K. Akiba, T. C. Kobayashi, H. T. Hirose and Z. Hiroi, J. Phys. Soc. Jpn. **89**, 114711 (2020).

3. †*Bulk quantum Hall effect of spin-valley coupled Dirac fermions in the polar antiferromagnet $BaMnSb_2$: H. Sakai, H. Fujimura, S. Sakuragi, M. Ochi, R. Kurihara, A. Miyake, M. Tokunaga, T. Kojima, D. Hashizume, T. Muro, K. Kuroda, T. Kondo, T. Kida, M. Hagiwara, K. Kuroki, M. Kondo, K. Tsuruda, H. Murakawa and N. Hanasaki, Phys. Rev. B **101**, 081104/1-7 (2020).

4. High-field ultrasonic study of quadrupole ordering and crystal symmetry breaking in $CeRhIn_5$: R. Kurihara, A. Miyake, M. Tokunaga, Y. Hirose and R. Settai, Phys. Rev. B **101**, 155125/1-8 (2020).

5. †Intriguing behavior of $UCo_{1-x}Rh_xGe$ ferromagnets in magnetic field along the axis: J. Pospíšil, Y. Haga, A. Miyake, S. Kambe, Y. Tokunaga, M. Tokunaga, E. Yamamoto, P. Proschek, J. Volný and V. Sechovský, Phys. Rev. B **102**, 024442/1-13 (2020).

6. Magnetic phase diagram enriched by chemical substitution in a noncentrosymmetric helimagnet: T. Sato, Y. Araki, A. Miyake, A. Nakao, N. Abe, M. Tokunaga, S. Kimura, Y. Tokunaga and T.-H. Arima, Phys. Rev. B **101**, 054414/1-6 (2020).

7. †Magnetic structures and quadratic magnetoelectric effect in $LiNiPO_4$ beyond 30 T: E. Fogh, T. Kihara, R. Toft-Petersen, M. Bartkowiak, Y. Narumi, O. Prokhnenko, A. Miyake, M. Tokunaga, K. Oikawa, M. K. Sørensen, J. C. Dyrnum, H. Grimmer, H. Nojiri and N. B. Christensen, Phys. Rev. B **101**, 024403/1-12 (2020).

8. *Magnetotransport properties of tellurium under extreme conditions: K. Akiba, K. Kobayashi, T. C. Kobayashi, R. Koezuka, A. Miyake, J. Gouchi, Y. Uwatoko and M. Tokunaga, Phys. Rev. B **101**, 245111(1-6) (2020).

9. †Metamagnetic transitions and magnetoelectric responses in the chiral polar helimagnet Ni_2InSbO_6: Y. Araki, T. Sato, Y. Fujima, N. Abe, M. Tokunaga, S. Kimura, D. Morikawa, V. Ukleev, Y. Yamasaki, C. Tabata, H. Nakao, Y. Murakami, H. Sagayama, K. Ohishi, Y. Tokunaga and T. Arima, Phys. Rev. B **102**, 054409/1-8 (2020).

10. †Strong magnetic anisotropy and unusual magnetic field reinforced phase in URhSn with a quasi-kagome structure: Y. Shimizu, A. Miyake, A. Maurya, F. Honda, A. Nakamura, Y. J. Sato, D. Li, Y. Homma, M. Yokoyama, Y. Tokunaga, M. Tokunaga and D. Aoki, Phys. Rev. B **102**, 134411/1-11 (2020).

11. *Anisotropic Fully Gapped Superconductivity Possibly Mediated by Charge Fluctuations in a Nondimeric Organic Complex: S. Imajo, H. Akutsu, R. Kurihara, T. Yajima, Y. Kohama, M. Tokunaga, K. Kindo and Y. Nakazawa, Phys. Rev. Lett. **125**, 177002 (2020).

12. †Dynamic evolution of flux distributions in a pulse-driven superconductor by high-speed magneto-optical imaging: H. Kurokawa, Y. Kinoshita, F. Nabeshima, M. Tokunaga and A. Maeda, Appl. Phys. Lett. **116**, 262601/1-5 (2020).

13. †*Synthesis, Structure, and Anomalous Magnetic Ordering of the Spin-1/2 Coupled Square Tetramer System $K(NbO)Cu_4(PO_4)_4$: K. Kimura, D. Urushihara, T. Asaka, M. Toyoda, A. Miyake, M. Tokunaga, A. Matsuo, K. Kindo, K. Yamauchi and T. Kimura, Inorg. Chem. **59**, 10986-10995 (2020).

14. Anisotropic Quantum Transport through a Single Spin Channel in the Magnetic Semiconductor $EuTiO_3$: K. Maruhashi, K. S. Takahashi, M. S. Bahramy, S. Shimizu, R. Kurihara, A. Miyake, M. Tokunaga, Y. Tokura and M. Kawasaki, Adv. Mater. **32**, 1908315/1-10 (2020).

15. †High-Mobility 2D Hole Gas at a $SrTiO_3$ Interface: L. D. Anh, S. Kaneta, M. Tokunaga, M. Seki, H. Tabata, M. Tanaka and S. Ohya, Adv. Mater. **32**, 1906003/1-7 (2020).

16. Magnetic field induced antiferromagnetic cone structure in multiferroic $BiFeO_3$: M. Matsuda, S. E. Dissanayake, T. Hong, Y. Ozaki, T. Ito, M. Tokunaga, X. Z. Liu, M. Bartkowiak and O. Prokhnenko, Phys. Rev. Materials **4**, 034412/1-6 (2020).

17. Capacitive detection of magnetostriction, dielectric constant, and magneto-caloric effects in pulsed magnetic fields: A. Miyake, H. Mitamura, S. Kawachi, K. Kimura, T. Kimura, T. Kihara, M. Tachibana and M. Tokunaga, Review of Scientific Instruments **91**, 105103/1-9 (2020).

18. *Improved accuracy in high-frequency AC transport measurements in pulsed high magnetic fields: H. Mitamura, R. Watanuki, E. Kampert, T. Förster, A. Matsuo, T. Onimaru, N. Onozaki, Y. Amou, K. Wakiya, K. T. Matsumoto, I. Yamamoto, K. Suzuki, S. Zherlitsyn, J. Wosnitza, M. Tokunaga, K. Kindo and T. Sakakibara, Review of Scientific Instruments **91**, 125107/1-25 (2020).

† Joint research with outside partners.

19. *Devil's staircase transition of the electronic structures in CeSb: K. Kuroda, Y. Arai, N. Rezaei, S. Kunisada, S. Sakuragi, M. Alaei, Y. Kinoshita, C. Bareille, R. Noguchi, M. Nakayama, S. Akebi, M. Sakano, K. Kawaguchi, M. Arita, S. Ideta, K. Tanaka, H. Kitazawa, K. Okazaki, M. Tokunaga, Y. Haga, S. Shin, H. S. Suzuki, R. Arita and T. Kondo, Nat Commun **11**, 2888/1-9 (2020).

20. †High-field magnetization and magnetic phase diagram of metamagnetic shape memory alloys Ni_{50}−Co $Mn_{31.5}Ga_{18.5}$ (x = 9 and 9.7): T. Kihara, X. Xu, A. Miyake, Y. Kinoshita, M. Tokunaga, Y. Adachi and T. Kanomata, Scripta Materialia **181**, 25-29 (2020).

21. †*Spin Excitations of the S = 1/2 One-Dimensional Ising-Like Antiferromagnet $BaCo_2V_2O_8$ in Transverse Magnetic Fields: A. Okutani, H. Onishi, S. Kimura, T. Takeuchi, T. Kida, M. Mori, A. Miyake, M. Tokunaga, K. Kindo and M. Hagiwara, J. Phys. Soc. Jpn. **90**, 044704/1-9 (2021).

22. †*Field-induced valence fluctuations in YbB_{12}: R. Kurihara, A. Miyake, M. Tokunaga, A. Ikeda, Y. H. Matsuda, A. Miyata, D. I. Gorbunov, T. Nomura, S. Zherlitsyn, J. Wosnitza and F. Iga, Phys. Rev. B **103**, 115103 1-14 (2021).

23. †*Geometrical Hall effect and momentum-space Berry curvature from spin-reversed band pairs: M. Hirschberger, Y. Nomura, H. Mitamura, A. Miyake, T. Koretsune, Y. Kaneko, L. Spitz, Y. Taguchi, A. Matsuo, K. Kindo, R. Arita, M. Tokunaga and Y. Tokura, Phys. Rev. B **103**, L041111(1-6) (2021).

24. †Martensitic Transformation and Metamagnetic Transition in Co-V-(Si, Al) Heusler Alloys: K. Nakamura, A. Miyake, X. Xu, T. Omori, M. Tokunaga and R. Kainuma, Metals **11**, 226/1-12 (2021).

25. †Observation of inverse magnetocaloric effect in magnetic-field-induced austenite phase of Heusler alloys $Ni_{50-x}Co_xMn_{31.5}Ga_{18.5}$ (x = 9 and 9.7): T. Kihara, T. Roy, X. Xu, A. Miyake, M. Tsujikawa, H. Mitamura, M. Tokunaga, Y. Adachi, T. Eto and T. Kanomata, Phys. Rev. Materials **5**, 034416_1-13 (2021).

26. †Giant anomalous Hall effect from spin-chirality scattering in a chiral magnet: Y. Fujishiro, N. Kanazawa, R. Kurihara, H. Ishizuka, T. Hori, F. S. Yasin, X. Yu, A. Tsukazaki, M. Ichikawa, M. Kawasaki, N. Nagaosa, M. Tokunaga and Y. Tokura, Nat Commun **12**, 317/1-6 (2021).

Y. Matsuda group

The magnetic-field-induced insulator to metal transition in W-doped VO_2 has been discovered in 500 T using the electromagnetic flux compression ultrahigh magnetic field generator, The molecular orbital is destabilized by such a strong magnetic field through the Pauli exclusion principle. This phenomenon can happen with the large spin Zeeman energy and the electron-electron correlation. In magnetic fields as high as 100 -200 T, we have investigated the magnon Bose-Einstein condensation in $TlCuCl_3$ and spin-state crystallization in $LaCoO_3$. As for technical achievements, a measurement technique for electric resistivity and a method for boosting magnetic field have been developed. Also, we have proposed a combination of 100 T magnetic fields and an intense x-ray by utilizing the single-turn coil method and the Japanese x-ray free electron laser SACLA. In addition, cyclotron resonance in an InAs quantum well, temperature dependent magnetization process in YbB_{12}, and magnetic properties in $Mn_2V_2O_7$ have been studied in high magnetic fields.

1. †*Experimental measurements of effective mass in near-surface InAs quantum wells: J. Yuan, M. Hatefipour, B. A. Magill, W. Mayer, M. C. Dartiailh, K. Sardashti, K. S. Wickramasinghe, G. A. Khodaparast, Y. H. Matsuda, Y. Kohama, Z. Yang, S. Thapa, C. J. Stanton and J. Shabani, Phys. Rev. B **101**, 205310 1-8 (2020).

2. †*Magnetization plateau observed by ultrahigh-field Faraday rotation in the kagome antiferromagnet herbertsmithite: R. Okuma, D. Nakamura and S. Takeyama, Phys. Rev. B **102**, 104429 1-4 (2020).

3. †Pressure and magnetic field effects on ferroelastic and antiferromagnetic orderings in honeycomb-lattice $Mn_2V_2O_7$: H. C. Wu, D. J. Hsieh, T. W. Yen, P. J. Sun, D. Chandrasekhar Kakarla, J. L. Her, Y. H. Matsuda, C. K. Chang, Y. C. Lai, M. Gooch, L. Z. Deng, K. G. Webber, C. A. Lee, M. M. C. Chou, C. W. Chu and H. D. Yang, Phys. Rev. B **102**, 075130 1-8 (2020).

4. †*Quantum limit cyclotron resonance in monolayer epitaxial graphene in magnetic fields up to 560 T: The relativistic electron and hole asymmetry: D. Nakamura, H. Saito, H. Hibino, K. Asano and S. Takeyama, Phys. Rev. B **101**, 115420 1-5 (2020).

5. †*Particle-Hole Symmetry Breaking in a Spin-Dimer System $TlCuCl_3$ Observed at 100 T: X. -G. Zhou, Y. Yao, Y. H. Matsuda, A. Ikeda, A. Matsuo, K. Kindo and H. Tanaka, Phys. Rev. Lett. **125**, 267207 1-6 (2020).

6. †Two Spin-State Crystallizations in $LaCoO_3$: A. Ikeda, Y. H. Matsuda and K. Sato, Phys. Rev. Lett. **125**, 177202 1-6 (2020).

7. †The Temperature Dependence of the Magnetization Process of the Kondo Insulator YbB_{12}: Y. H. Matsuda, Y. Kakita

* Joint research among groups within ISSP.

and F. Iga, Crystals **10**, 26 1-7 (2020).

8. †*Direct measurement of resistivity in destructive pulsed magnetic fields: Y. Kohama, F. Nabeshima, A. Maeda, A. Ikeda and Y. H. Matsuda, Review of Scientific Instruments **91**, 033901 1-5 (2020).

9. †*Magnetic-field-induced insulator–metal transition in W-doped VO_2 at 500 T: Y. H. Matsuda, D. Nakamura, A. Ikeda, S. Takeyama, Y. Suga, H. Nakahara and Y. Muraoka, Nat Commun **11**, 3591 1-7 (2020).

10. †*Single shot x-ray diffractometry in SACLA with pulsed magnetic fields up to 16 T: A. Ikeda, Y. H. Matsuda, X. Zhou, T. Yajima, Y. Kubota, K. Tono and M. Yabashi, Phys. Rev. Research **2**, 043175 1-6 (2020).

11. †*Field-induced valence fluctuations in YbB_{12}: R. Kurihara, A. Miyake, M. Tokunaga, A. Ikeda, Y. H. Matsuda, A. Miyata, D. I. Gorbunov, T. Nomura, S. Zherlitsyn, J. Wosnitza and F. Iga, Phys. Rev. B **103**, 115103 1-14 (2021).

12. †*Higher magnetic-field generation by a mass-loaded single-turn coil: M. Gen, A. Ikeda, S. Kawachi, T. Shitaokoshi, Y. H. Matsuda, Y. Kohama and T. Nomura, Review of Scientific Instruments **92**, 033902 1-5 (2021).

Kohama group

In 2020, we have investigated high-field properties in many different systems, such as $CeRhIn_5$, $SrRuO_3$, $CuInCr_4S_8$, FeSe, Ruby, High-Tc superconductor, and so on. We also developed the resistivity measurment technique for a research in ultra high-magnetic fields above 100 T. The other technical developments including the super-capacitor driven pulsed magnet are underway.

1. †Symmetry Lowering on the Field-Induced Commensurate Phase in $CeRhIn_5$: T. Kanda, K. Arashima, Y. Hirose, R. Settai, K. Matsui, T. Nomura, Y. Kohama and Y. Ihara, J. Phys. Soc. Jpn. **89**, 094709 (2020).

2. Electronic band structure of (111) SrRuO3 thin films: An angle-resolved photoemission spectroscopy study: H. Ryu, Y. Ishida, B. Kim, J. R. Kim, W. J. Kim, Y. Kohama, S. Imajo, Z. Yang, W. Kyung, S. Hahn, B. Sohn, I. Song, M. Kim, S. Huh, J. Jung, D. Kim, T. W. Noh, S. Das and C. Kim, Phys. Rev. B **102**, 041102 (2020).

3. *Enhanced spin correlations in the Bose-Einstein condensate compound $Sr_3Cr_2O_8$: T. Nomura, Y. Skourski, D. L. Quintero-Castro, A. A. Zvyagin, A. V. Suslov, D. Gorbunov, S. Yasin, J. Wosnitza, K. Kindo, A. T. M. N. Islam, B. Lake, Y. Kohama, S. Zherlitsyn and M. Jaime, Phys. Rev. B **102**, 165144 (2020).

4. †*Experimental measurements of effective mass in near-surface InAs quantum wells: J. Yuan, M. Hatefipour, B. A. Magill, W. Mayer, M. C. Dartiailh, K. Sardashti, K. S. Wickramasinghe, G. A. Khodaparast, Y. H. Matsuda, Y. Kohama, Z. Yang, S. Thapa, C. J. Stanton and J. Shabani, Phys. Rev. B **101**, 205310 1-8 (2020).

5. Magnetization process of the breathing pyrochlore magnet $CuInCr_4S_8$ in ultrahigh magnetic fields up to 150 T: M. Gen, Y. Okamato, M. Mori, K. Takenaka and Y. Kohama, Phys. Rev. B **101**, 054434 (2020).

6. *Observation of in-plane magnetic field induced phase transitions in FeSe: J. M. Ok, C. I. Kwon, Y. Kohama, J. S. You, S. K. Park, J.-H. Kim, Y. J. Jo, E. S. Choi, K. Kindo, W. Kang, K.-S. Kim, E. G. Moon, A. Gurevich and J. S. Kim, Phys. Rev. B **101**, 224509 (2020).

7. *Quantum oscillations and magnetic field induced Fermi surface reconstruction in the charge density wave state of $A_{0.9}Mo_6O_{17}$ (A = Na, K): H. P. Zhu, M. Yang, J. Z. Ke, H. K. Zuo, T. Peng, J. F. Wang, Y. Liu, X. Xu, Y. Kohama, K. Kindo and M. Greenblatt, Phys. Rev. B **102**, 235164 (2020).

8. *Anisotropic Fully Gapped Superconductivity Possibly Mediated by Charge Fluctuations in a Nondimeric Organic Complex: S. Imajo, H. Akutsu, R. Kurihara, T. Yajima, Y. Kohama, M. Tokunaga, K. Kindo and Y. Nakazawa, Phys. Rev. Lett. **125**, 177002 (2020).

9. *Observation of small Fermi pockets protected by clean CuO_2 sheets of a high-Tc superconductor: S. Kunisada, S. Isono, Y. Kohama, S. Sakai, C. Bareille, S. Sakuragi, R. Noguchi, K. Kurokawa, K. Kuroda, Y. Ishida, S. Adachi, R. Sekine, T. K. Kim, C. Cacho, S. Shin, T. Tohyama, K. Tokiwa and T. Kondo, Science **369**, 833 (2020).

10. *Extracting the Chiral Contribution to the Negative Longitudinal Magnetoresistance in Epitaxial $Pr_2Ir_2O_7$ Thin Films: T. Ohtsuki, Z. Tian, A. Endo, M. Halim, S. Katsumoto, Y. Kohama, K. Kindo, M. Lippmaa and S. Nakatsuji, JPS Conf. Proc. **30**, 011181 (1-6) (2020).

11. Strain engineering of the magnetic multipole moments and anomalous Hall effect in pyrochlore iridate thin films: W. J. Kim, T. Oh, J. Song, E. K. Ko, Y. Li, J. Mun, B. Kim, J. Son, Z. Yang, Y. Kohama, M. Kim, B.-J. Yang and T. W. Noh, Sci. Adv. **6**, eabb1539 (2020).

12. †*Direct measurement of resistivity in destructive pulsed magnetic fields: Y. Kohama, F. Nabeshima, A. Maeda,

† Joint research with outside partners.

A. Ikeda and Y. H. Matsuda, Review of Scientific Instruments **91**, 033901 1-5 (2020).

13. Angle dependence of H_{c2} with a crossover between the orbital and paramagnetic limits: H. Matsuoka, M. Nakano, T. Shitaokoshi, Y. Wang, Y. Kashiwabara, S. Yoshida, Y. Kohama, T. Ouchi, K. Ishizaka, M. Kawasaki, T. Nojima and Y. Iwasa, Phys. Rev. Research **2**, 012064(R) (2020).

14. Crystal-field Paschen-Back effect on ruby in ultrahigh magnetic fields: M. Gen, T. Kanda, T. Shitaokoshi, Y. Kohama and T. Nomura, Phys. Rev. Research **2**, 033257 (2020).

15. Van der Waals $SnSe_{2(1-x)}S_{2x}$ Alloys: Composition-Dependent Bowing Coefficient and Electron–Phonon Interaction: Z. R. Kudrynskyi, X. Wang, J. Sutcliffe, M. A. Bhuiyan, Y. Fu, Z. Yang, O. Makarovsky, L. Eaves, A. Solomon, V. T. Maslyuk, Z. D. Kovalyuk, L. Zhang and A. Patanè, Advanced Functional Materials **30**, 1908092 (2020).

16. Broad Tunability of Carrier Effective Masses in Two-Dimensional Halide Perovskites: M. Dyksik, H. Duim, X. Zhu, Z. Yang, M. Gen, Y. Kohama, S. Adjokatse, D. K. Maude, M. A. Loi, D. A. Egger, M. Baranowski and P. Plochocka, ACS Energy Lett. **5**, 3609 (2020).

17. *High-field phase diagram of $Ni_3V_2O_8$ studied by specific heat and magnetocaloric effect measurements: C. Dong, Y. Kohama, Z. Z. He, X. T. Han, K. Sato, A. Matsuo, K. Kindo, M. Yang and J. F. Wang, J. Phys.: Condens. Matter **33**, 205402 (2021).

18. Emergence of Frustrated Short-Range Order above Long-Range Order in the S = 1/2 Kagome Antiferromagnet $CaCu_3(OD)_6Cl_2 \cdot 0.6D_2O$: Y. Ihara, K. Matsui, Y. Kohama, S. Luther, D. Opherden, J. Wosnitza, H. Kühne and H. K. Yoshida, J. Phys. Soc. Jpn. **90**, 023703 (2021).

19. Element-specific field-induced spin reorientation and tetracritical point in $MnCr_2S_4$: Sh. Yamamoto, H. Suwa, T. Kihara, T. Nomura, Y. Kotani, T. Nakamura, Y. Skourski, S. Zherlitsyn, L. Prodan, V. Tsurkan, H. Nojiri, A. Loidl and J. Wosnitza, Phys. Rev. B **103**, L020408 (2021).

20. Wide Critical Fluctuations of the Field-Induced Phase Transition in Graphite: C. Marcenat, T. Klein, D. LeBoeuf, A. Jaoui, G. Seyfarth, J. Kacmarcik, Y. Kohama, H. Cercellier, H. Aubin, K. Behnia and B. Fauque, Phys. Rev. Lett. **126**, 106801 (2021).

21. *Compact megajoule-class pulsed power supply for generating long-pulsed magnetic fields: K. Matsui, T. Kanda, Y. Ihara, K. Kindo and Y. Kohama, Review of Scientific Instruments **92**, 024711 (2021).

22. †*Higher magnetic-field generation by a mass-loaded single-turn coil: M. Gen, A. Ikeda, S. Kawachi, T. Shitaokoshi, Y. H. Matsuda, Y. Kohama and T. Nomura, Review of Scientific Instruments **92**, 033902 1-5 (2021).

23. *High-resolution calorimetry in pulsed magnetic fields: S. Imajo, C. Dong, A. Matsuo, K. Kindo and Y. Kohama, Review of Scientific Instruments **92**, 043901 (2021).

Center of Computational Materials Science

Akai team

The main objective of is to predict/discover new functionality materials by means of computational materials design (CMD). In particular, new high-performance permanent magnets is one of main targets. Developments of new methods of quantum simulation are also important themes. Our activities include the followings: (1) A method that enabled us to treat low energy collective excitations, phonons and magnons, in the framework of first-principles KKR-CPA was developed and applied to various magnetic systems. The effects of these excitations on magnetization at finite temperature and the Curie temperature of typical magnetic systems, including bcc Fe and permanent-magnet materials $B_2(Fe, Co)_{14}B$, were calculated using low energy effective Hamiltonian obtained by a first-principles KKR-Green's function method where the magnons and phonons were included in a static and local scheme. The effects of these excitations were important in determining the magnetic properties, was concluded; (2) The magnetic Friedel oscillation near the surface of Fe films was detected layer by layer measurement using synchrotron Mössbauer source. The behavior was well reproduced by the hyperfine interactions calculated using the full-potential KKR method and the KKR method combined the optimized effective potential (OEP) method; (3) An efficient method to calculate spin-wave dispersions using the low-energy effective Hamiltonian derived from first-principles calculations was developed and applied to rare-earth based permanent magnet materials including $R_2(Fe, Co)_{14}B$; (4) A search for rare-earth bases permanent magnets materials of better performance at finite temperature were made using massive data obtained as results of first-principles KKR-CPA together with fairly large number of experimental data by a newly developed data assimilation technique. The method developed was proven powerful enough to predict possible candidates for compositions of high-performance permanent magnet materials.

* Joint research among groups within ISSP.

1. Calculating Curie temperatures for rare-earth permanent magnets: *Ab initio* inspection of localized magnetic moments in *d*-electron ferromagnetism: M. Matsumoto and H. Akai, Phys. Rev. B **101**, 144402 (2020).

2. Element- and orbital-selective magnetic coherent rotation at the first-order phase transition of a hard uniaxial ferrimagnet: Sh. Yamamoto, D. I. Gorbunov, H. Akai, H. Yasumura, Y. Kotani, T. Nakamura, T. Kato, N. V. Mushnikov, A. V. Andreev, H. Nojiri and J. Wosnitza, Phys. Rev. B **101**, 174430 (2020).

3. Magnetic Friedel Oscillation at the Fe(001) Surface: Direct Observation by Atomic-Layer-Resolved Synchrotron Radiation ^{57}Fe Mössbauer Spectroscopy: T. Mitsui, S. Sakai, S. Li, T. Ueno, T. Watanuki, Y. Kobayashi, R. Masuda, M. Seto and H. Akai, Phys. Rev. Lett. **125**, 236806 (2020).

4. [*]First-principles calculations of finite temperature electronic structures and transport properties of Heusler alloy Co_2MnSi: H. Shinya, S. Kou, T. Fukushima, A. Masago, K. Sato, H. Katayama-Yoshida and H. Akai, Appl. Phys. Lett. **117**, 042402(1-5) (2020).

5. Spin-wave dispersion and exchange stiffness in $Nd_2Fe_{14}B$ and $RFe_{11}Ti$ (R=Y, Nd, Sm) from first-principles calculations: T. Fukazawa, H. Akai, Y. Harashima and T. Miyake, Phys. Rev. B **103**, 024418-1–7 (2021).

6. Data assimilation method for experimental and first-principles data: Finite-temperature magnetization of (Nd, Pr, La, Ce)$_2$(Fe, Co, Ni)$_{14}$B: Y. Harashima, K. Tamai, S. Doi, M. Matsumoto, H. Akai, N. Kawashima, M. Ito, N. Sakuma, A. Kato, T. Shoji and T. Miyake, Phys. Rev. Materials **5**, 013806-1–10 (2021).

Miyashita team

We studied temperature dependence of coercivity for permanent magnets as the activity of ESICMM. We also studied subjects for phase transitions and quantum dynamics.

1. Dynamical aspects of magnetization reversal in the neodymium permanent magnet by a stochastic Landau-Lifshitz-Gilbert simulation at finite temperature: Real-time dynamics and quantitative estimation of coercive force: M. Nishino, I. E. Uysal, T. Hinokihara and S. Miyashita, Phys. Rev. B **102**, 020413(R) (1-5) (2020).

2. Elastic-frustration-driven unusual magnetoelastic properties in a switchable core-shell spin-crossover nanostructure: Y. Singh, H. Oubouchou, M. Nishino, S. Miyashita and K. Boukheddaden, Phys. Rev. B **101**, 054105(1-15) (2020).

3. Magnetic field threshold for nucleation and depinning of domain walls in the neodymium permanent magnet $Nd_2Fe_{14}B$: I. E. Uysal, M. Nishino and S. Miyashita, Phys. Rev. B **101**, 094421 (1-9) (2020).

4. Dynamical phase transition in Floquet optical bistable systems: An approach from finite-size quantum systems: T. Shirai, S. Todo and S. Miyashita, Phys. Rev. E **101**, 013809(1-7) (2020).

5. Magnetic-Pole Flip by Millimeter Wave: S.-I. Ohkoshi, M. Yoshikiyo, K. Imoto, K. Nakagawa, A. Namai, H. Tokoro, Y. Yahagi, K. Takeuchi, F. Jia, S. Miyashita, M. Nakajima, H. Qiu, K. Kato, T. Yamaoka, M. Shirata, K. Naoi, K. Yagishita and H. Doshita, Adv. Mater. **32**, 2004897(1-7) (2020).

6. Construction of quantum dark soliton in onedimensional Bose gas: E. Kaminishi, T. Mori and S. Miyashita, J. Phys. B: At. Mol. Opt. Phys. **53**, 095302(1-8) (2020).

7. Role of atomic-scale thermal fluctuations in the coercivity: Y. Toga, S. Miyashita, A. Sakuma and T. Miyake, npj Computational Materials **6:67**, 1-7 (2020).

8. Effect of the surface magnetic anisotropy of neodymium atoms on the coercivity in neodymium permanent magnets: M. Nishino, I. E. Uysal and S. Miyashita, Phys. Rev. B **103**, 014418(1-9) (2021).

9. Systematic survey of magnetic configurations in multilayer ferromagnet system with dipole-dipole interaction: T. Hinokihara and S. Miyashita, Phys. Rev. B **103**, 054421(1-9) (2021).

10. Rapid Faraday Rotation on epsilon-Iron Oxide Magnetic Nanoparticles by Visible and Terahertz Pulsed Light: S.-I. Ohkoshi, K. Imoto, A. Namai, M. Yoshikiyo, S. Miyashita, H. Qiu, S. Kimoto, K. Kato and M. Nakajima, J. Am. Chem. Soc. **141**, 1775-1780 (2021).

† Joint research with outside partners.

Laser and Synchrotron Research Center

Kobayashi group

We have supplied some laser systems for applications such as astronomical science and photoemission spectroscopy. Some results related to a laser processing were published in 2020.

1. †Ablation threshold and crater morphology of amorphous and crystalline SiO_2 glass for extreme ultraviolet femtosecond pulses: T. Shibuya, K. Sakaue, H. Ogawa, T. -H. Dinh, D. Satoh, E. Terasawa, M. Washio, M. Tanaka, T. Higashiguchi, M. Ishino, Y. Kubota, Y. Inubushi, S. Owada, M. Nishikino, Y. Kobayashi and R. Kuroda, Jpn. J. Appl. Phys. **59**, 122004 (2020).

2. †Precision measurement of ablation thresholds with variable pulse duration laser: T. Takahashi, S. Tani, R. Kuroda and Y. Kobayashi, Appl. Phys. A **126**, 582 (2020).

3. †Study on nonthermal–thermal processing boundary in drilling of ceramics using ultrashort pulse laser system with variable parameters over a wide range: A. Narazaki, H. Takada, D. Yoshitomi, K. Torizuka and Y. Kobayashi, Appl. Phys. A **126**, 252 (2020).

4. レーザーアブレーションの学理解明と次世代レーザー加工に向けた自動計測技術開発：小林 洋平 , 高橋 孝 , 谷峻 太郎 , 応用物理 **, Vol.89, No.12**, 719-723 (2020).

5. *Q*-switching stability limits of Kerr-lens mode locking: S. Kimura, S. Tani and Y. Kobayashi, Phys. Rev. A **102**, 043505 (2020).

6. Neural-network-assisted in situ processing monitoring by speckle pattern observation: S. Tani, Y. Aoyagi and Y. Kobayashi, Opt. Express **28**, 26180 (2020).

7. Piezo-electric transducer actuated mirror with a servo bandwidth beyond 500 kHz: T. Nakamura, S. Tani, I. Ito, M. Endo and Y. Kobayashi, Opt. Express **28**, 16118 (2020).

8. †Work function seen with sub-meV precision through laser photoemission: Y. Ishida, J. K. Jung, M. S. Kim, J. Kwon, Y. S. Kim, D. Chung, I. Song, C. Kim, T. Otsu and Y. Kobayashi, Commun Phys **3**, 158 (2020).

9. Subgigahertz-resolution table-top spectrograph calibrated with a 4-GHz optical frequency comb: M. Endo, T. Sukegawa, A. Silva and Y. Kobayashi, J. Astron. Telesc. Instrum. Syst. **6**, 1 (2020).

10. †Ablation thresholds and morphological changes of poly-L-lactic acid for pulse durations in the femtosecond-to-picosecond regime: T. Shibuya, D. Yoshitomi, D. Satoh, K. Sakaue, M. Tanaka, H. Takada, H. Ogawa, K. Torizuka, Y. Kobayashi and R. Kuroda, Surf Interface Anal **52**, 1145 (2020).

11. 固体レーザーによる光周波数コム：小林 洋平 , 木村 祥太 , 電子情報通信学会誌 , **Vol.103, No.11**, 1082, 1088 (2020).

12. *Direct generation of sub-picosecond pulse via multi-section gain switching: T. Nakamura, T. Ito, H. Nakamae, C. Kim, Y. Hazama, Y. Kobayashi, R. Kuroda and H. Akiyama, Opt. Lett. **46**, 1277 (2021).

13. Coherent control of acoustic phonons in a silica fiber using a multi-GHz optical frequency comb: M. Endo, S. Kimura, S. Tani and Y. Kobayashi, Commun Phys **4**, 73 (2021).

14. †Ultrafast laser processing of ceramics: Comprehensive survey of laser parameters: A. Narazaki, H. Takada, D. Yoshitomi, K. Torizuka and Y. Kobayashi, Journal of Laser Applications **33**, 012009 (2021).

Harada group

This year, in order to tackle the new coronavirus problem, we analyzed water treatment membranes that can be used as virus removal membranes as part of the project to analyze the solid-liquid interface, which is the main theme of Grant-in-Aid for Scientific Research on Innovative Areas "Aquatic Functional Materials". With the support of the AMED project "Development of Technology for Countermeasures against Infectious Diseases including Viruses," we also promoted research and development on the improvement of coating materials for the inner wall of the tubes for Extra Corporeal Membrane Oxygenation (ECMO), which is mainly used in the treatment of patients with severe pneumonia. In order to develop cathode materials that contribute to the high performance of lithium-ion batteries, we analyzed materials in which the ligand oxygen, rather than transition metals, is involved in the redox reaction. We succeeded in capturing the dimerization of oxygen atoms interacting with metals under high potentials using RIXS.

1. †Revisiting the Phase Diagram of T*-type $La_{1-x/2}Eu_{1-x/2}Sr_xCuO_4$ Using Oxygen K-edge X-ray Absorption Spectroscopy: S. Asano, K. Ishii, K. Yamagami, J. Miyawaki, Y. Harada and M. Fujita, J. Phys. Soc. Jpn. **89**, 075002 (1-2)

* Joint research among groups within ISSP.

(2020).

2. †*Localized character of charge excitations for $La_{2-x}Sr_xNiO_{4+\delta}$ revealed by oxygen K-edge resonant inelastic x-ray scattering: K. Yamagami, K. Ishii, Y. Hirata, K. Ikeda, J. Miyawaki, Y. Harada, M. Miyazaki, S. Asano, M. Fujita and H. Wadati, Phys. Rev. B **102**, 165145 (1-7) (2020).

3. †Anisotropic X-Ray Scattering of Transiently Oriented Water: K. H. Kim, A. Späh, H. Pathak, C. Yang, S. Bonetti, K. Amann-Winkel, D. Mariedahl, D. Schlesinger, J. A. Sellberg, D. Mendez, G. van der Schot, H. Y. Hwang, J. Clark, O. Shigeki, T. Tadashi, Y. Harada, H. Ogasawara, T. Katayama, A. Nilsson and F. Perakis, Phys. Rev. Lett. **125**, 076002 (1-6) (2020).

4. †Ion Selectivity of Water Molecules in Subnanoporous Liquid-Crystalline Water-Treatment Membranes: A Structural Study of Hydrogen Bonding: R. Watanabe, T. Sakamoto, K. Yamazoe, J. Miyawaki, T. Kato and Y. Harada, Angew. Chem. Int. Ed. **59**, 23461-23465 (2020).

5. †Tetragonal Distortion of a $BaTiO_3/Bi_{0.5}Na_{0.5}TiO_3$ Nanocomposite Responsible for Anomalous Piezoelectric and Ferroelectric Behaviors: W. Zhang, Q. Feng, E. Hosono, D. Asakura, J. Miyawaki and Y. Harada, ACS Omega **5**, 22800-22807 (2020).

6. †Multiorbital bond formation for stable oxygen-redox reaction in battery electrodes: T. Sudayama, K. Uehara, T. Mukai, D. Asakura, X.-M. Shi, A. Tsuchimoto, B. M. D. Boisse, T. Shimada, E. Watanabe, Y. Harada, M. Nakayama, M. Okubo and A. Yamada, Energy Environ. Sci. **13**, 1492-1500 (2020).

I. Matsuda group

Since the beginning of the year 2020, there has been a serious coronavirus (COVID-19) pandemic over the world and care has been urgently needed for those affected. In living, we have had to stop the spread of the virus by avoiding three Cs: closed spaces, crowded places, and close contact. No exception has been applied for experiments in any facilities or laboratories, including our beamline, SPring-8 BL07LSU. A number of the user-group members and visiting itself have been restricted. After summer, beamtime experiments were carried out normally for domestic users. We have made advanced X-ray magneto-optical experiments of exotic quantum phases and ambient pressure photoemission measurements on surface reactions. In the laboratory, soft X-ray non-linear optical research was made at X-ray free electron laser facility at SACLA.

1. Topological Dirac nodal loops in nonsymmorphic hydrogenated monolayer boron: N. T. Cuong, I. Tateishi, M. Cameau, M. Niibe, N. Umezawa, B. Slater, K. Yubuta, T. Kondo, M. Ogata, S. Okada and I. Matsuda, Phys. Rev. B **101**, 195412 (2020).

2. Two-dimensional conducting layer on $SrTiO_3$ surface induced by hydrogenation: Y. Takeuchi, R. Hobara, R. Akiyama, A. Takayama, S. Ichinokura, R. Yukawa, I. Matsuda and S. Hasegawa, Phys. Rev. B **101**, 085422-1,-6 (2020).

3. †Time-resolved X-ray photoelectron diffraction using an angle-resolved time-of-flight electron analyzer: A. K. R. Ang, Y. Fukatsu, K. Kimura, Y. Yamamoto, T. Yonezawa, H. Nitta, A. Fleurence, S. Yamamoto, I. Matsuda, Y. Yamada-Takamura and K. Hayashi, Jpn. J. Appl. Phys. **59**, 100902 (2020).

4. *Element-selectively tracking ultrafast demagnetization process in Co/Pt multilayer thin films by the resonant magneto-optical Kerr effect: K. Yamamoto, S. E. Moussaoui, Y. Hirata, S. Yamamoto, Y. Kubota, S. Owada, M. Yabashi, T. Seki, K. Takanashi, I. Matsuda and H. Wadati, Appl. Phys. Lett. **116**, 172406-1,-5 (2020).

5. Scanning magneto-optical Kerr effect (MOKE) measurement with element-selectivity by using a soft x-ray free-electron laser and an ellipsoidal mirror: Y. Kubota, H. Motoyama, G. Yamaguchi, S. Egawa, Y. Takeo, M. Mizuguchi, H. Sharma, S. Owada, K. Tono, H. Mimura, I. Matsuda and M. Yabashi, Appl. Phys. Lett. **117**, 042405 (2020).

6. *A computational examination of the electric-field-induced proton transfer along the interface hydrogen bond between proton donating and accepting self-assembled monolayers: Y. Kanematsu, H. S. Kato, S. Yoshimoto, A. Ueda, S. Yamamoto, H. Mori, J. Yoshinobu, I. Matsuda and M. Tachikawa, Chem. Phys. Lett. **741**, 137091 (2020).

7. 分割型アンジュレータを用いた新しい軟 X 線磁気光学法と次世代光源への展開： 久保田 雄也， 松田 巌， 放射光 **33**, 206-212 (2020).

8. †*Atomistic-Level Description of GaN/Water Interface by a Combined Spectroscopic and First-Principles Computational Approach: M. Sato, Y. Imazeki, T. Takeda, M. Kobayashi, S. Yamamoto, I. Matsuda, J. Yoshinobu, Y. Nakano and M. Sugiyama, J. Phys. Chem. C **124**, 12466 (2020).

9. *Edge-state correlation accelerates metal-insulator transition in topological semimetal nanofilms: S. Ito, M. Arita, J. Haruyama, B. Feng, W. -C. Chen, H. Namatame, M. Taniguchi, C. -M. Cheng, G. Bian, S. -J. Tang, T. -C. Chiang, O. Sugino, F. Komori and I. Matsuda, Science Advances **6**, eaaz5015 (7 pages) (2020).

† Joint research with outside partners.

10. *Electronic structure of a (3×3)-ordered silicon layer on Al(111): Y. Sato, Y. Fukaya, M. Cameau, A. K. Kundu, D. Shiga, R. Yukawa, K. Horiba, C.-H. Chen, A. Huang, H.-T. Jeng, T. Ozaki, H. Kumigashira, M. Niibe and I. Matsuda, Phys. Rev. Materials **4**, 064005 (2020).

11. Ellipsometer Equipped with Multiple Mirrors for Element-selective Soft X-ray Experiments: M. Araki, J. Meikaku, Y. Kubota, J. Miyawaki, Y. Kosegawa, S. E. Moussaoui, T. Bouillaud, P. Manset, S. Owada, K. Tono, M. Yabashi and I. Matsuda, e-J. Surf. Sci. Nanotechnol. **18**, 231 (2020).

12. Geometrical Frustration of B-H Bonds in Layered Hydrogen Borides Accessible by Soft Chemistry: S. Tominaka, R. Ishibiki, A. Fujino, K. Kawakami, K. Ohara, I. Matsuda, H. Hosono and T. Kondo, Chem **6**, 406-418 (2020).

13. Recent progresses in spectroscopies using soft X-ray free-electron laser: I. Matsuda and Y. Kubota, Chem. Lett. **Advanced publication**, cl.200881 (2021).

14. †*Femtosecond Charge Density Modulations in Photoexcited $CuWO_4$: Y. Uemura, A. S. M. Ismail, S. H. Park, S. Kwon, M. Kim, Y. Niwa, H. Wadati, H. Elnaggar, F. Frati, T. Haarman, N. Höppel, N. Huse, Y. Hirata, Y. Zhang, K. Yamagami, S. Yamamoto, I. Matsuda, T. Katayama, T. Togashi, S. Owada, M. Yabashi, U. Halisdemir, G. Koster, T. Yokoyama, B. M. Weckhuysen and F. M. F. D. Groot, J. Phys. Chem. C **125**, 7329 (2021).

15. †Valence Fluctuations in Yb(Al,Fe)B_4 Studied by Nanosecond-time-resolved Photoemission Spectroscopy Using Synchrotron Radiation: M. Okawa, K. Akikubo, S. Yamamoto, I. Matsuda and T. Saitoh, e-J. Surf. Sci. Nanotechnol. **19**, 20 (2021).

Itatani group

We mainly worked on soft-X-ray attosecond spectroscopy and the upgrade of the attosecond beamline. First, we extended the nitrogen *K*-edge experiments from diatomic molecules (NO) to triatomic molecules (N_2O) and observed intriguing dynamics of 2ω oscillation. The interpretation of this ultrafast oscillation is underway. Second, a new sample-feeding system for organic molecules was introduced. We successfully measured static absorption spectra of benzene, acetone, ethanol, and methanol at the carbon *K* edge around 280 eV. Third, a new soft X-ray spectrometer was developed and installed to improve the energy resolution. In addition, we started to develop new infrastructures in the building E. We constructed a beamline booth next to the existing laser booth, with a clean and temperature-stable environment for ultrafast experiments using EUV and soft-X-ray pulses. A Ti:sapphire laser system was developed as a pump source for an ultrashort-pulse infrared optical parametric chirped pulse amplifier (OPCPA), or as a driver to produce high-flux femtosecond EUV pulses for imaging experiments. We also developed prototype light sources such as a mid-infrared optical parametric amplifier (OPA) and a harmonic-based tunable UV source, both of which are pumped by a high-repetition-rate Yb laser.

1. †*Photoinduced Phase Transition from Excitonic Insulator to Semimetal-like State in $Ta_2Ni_{1-x}Co_xSe_5$(x = 0.10): T. Mitsuoka, T. Suzuki, H. Takagi, N. Katayama, H. Sawa, M. Nohara, M. Watanabe, J. Xu, Q. Ren, M. Fujisawa, T. Kanai, J. Itatani, S. Shin, K. Okazaki and T. Mizokawa, J. Phys. Soc. Jpn. **89**, 124703 (2020).

2. †Detecting electron-phonon coupling during photoinduced phase transition,: T. Suzuki, Y. Shinohara, Y. Lu, M. Watanabe, J. Xu, K. L. Ishikawa, H. Takagi, M. Nohara, N. Katayama, H. Sawa, M. Fujisawa, T. Kanai, J. Itatani, T. Mizokawa, S. Shin and K. Okazaki, Phys. Rev. B **103**, L121105 (2020).

3. *Efficient Terahertz Harmonic Generation with Coherent Acceleration of Electrons in the Dirac Semimetal Cd_3As_2: B. Cheng, N. Kanda, T. N. Ikeda, T. Matsuda, P. Xia, T. Schumann, S. Stemmer, J. Itatani, N. P. Armitage and R. Matsunaga, Phys. Rev. Lett. **124**, 117402 (2020).

4. 軟 X 線領域でのアト秒分光 : 斎藤 成之 , 光学 **49**, 249 (2020).

5. 中赤外光パルスを用いた固体高次高調波発生とその偏光特性 : 石井 順久 , 金島 圭佑 , 夏 沛宇 , 斎藤 成之 , 金井 輝人 , 板谷 治郎 , レーザー研究 **49**, 168-173 (2020).

6. †Role of virtual band population for high harmonic generation in solids: Y. Sanari, H. Hirori, T. Aharen, H. Tahara, Y. Shinohara, K. L. Ishikawa, T. Otobe, P. Xia, N. Ishii, J. Itatani, S. A. Sato and Y. Kanemitsu, Phys. Rev. B (Rapid Communication) **102**, 041125(R)-1-7 (2020).

7. †Observation of the quantum shift of a backward rescattering caustic by carrier-envelope phase mapping: T. Mizuno, N. Ishii, T. Kanai, P. Rosenberger, D. Zietlow, M. F. Kling, O. I. Tolstikhin, T. Morishita and J. Itatani, Phys. Rev. A **103**, 043121 (2021).

8. *Optical parametric amplification of phase-stable terahertz-to-mid-infrared pulses studied in the time domain: N. Kanda, N. Ishii, J. Itatani and R. Matsunaga, Optics Express **29**, 3479-3489 (2021).

9. †Time-domain spectroscopy of optical parametric amplification for phase-stable terahertz-to-midinfrared pulses:

* Joint research among groups within ISSP.

N. Kanda, N. Ishii, J. Itatani and R. Matsunaga, Optics Express **29(3)**, 3479-3489 (2021).

Kondo group

We use angle-resolved photoemission spectroscopy (ARPES) with ultrahigh energy resolution. The main findings in 2020 were small pockets in cuprate, Devil's staircase in CeSb, and spin-polarized band in Te.

1. †*Bulk quantum Hall effect of spin-valley coupled Dirac fermions in the polar antiferromagnet BaMnSb2: H. Sakai, H. Fujimura, S. Sakuragi, M. Ochi, R. Kurihara, A. Miyake, M. Tokunaga, T. Kojima, D. Hashizume, T. Muro, K. Kuroda, T. Kondo, T. Kida, M. Hagiwara, K. Kuroki, M. Kondo, K. Tsuruda, H. Murakawa and N. Hanasaki, Phys. Rev. B **101**, 081104/1-7 (2020).

2. Three-dimensional electronic structure in ferromagnetic Fe_3Sn_2 with breathing kagome bilayers: H. Tanaka, Y. Fujisawa, K. Kuroda, R. Noguchi, S. Sakuragi, C. Bareille, B. Smith, C. Cacho, S. W. Jung, T. Muro, Y. Okada and T. Kondo, Phys. Rev. B **101**, 161114 (2020).

3. *Radial Spin Texture in Elemental Tellurium with Chiral Crystal Structure: M. Sakano, M. Hirayama, T. Takahashi, S. Akebi, M. Nakayama, K. Kuroda, K. Taguchi, T. Yoshikawa, K. Miyamoto, T. Okuda, K. Ono, H. Kumigashira, T. Ideue, Y. Iwasa, N. Mitsuishi, K. Ishizaka, S. Shin, T. Miyake, S. Murakami, T. Sasagawa and T. Kondo, Phys. Rev. Lett. **124**, 136404 (2020).

4. *Observation of small Fermi pockets protected by clean CuO_2 sheets of a high-Tc superconductor: S. Kunisada, S. Isono, Y. Kohama, S. Sakai, C. Bareille, S. Sakuragi, R. Noguchi, K. Kurokawa, K. Kuroda, Y. Ishida, S. Adachi, R. Sekine, T. K. Kim, C. Cacho, S. Shin, T. Tohyama, K. Tokiwa and T. Kondo, Science **369**, 833 (2020).

5. *Devil's staircase transition of the electronic structures in CeSb: K. Kuroda, Y. Arai, N. Rezaei, S. Kunisada, S. Sakuragi, M. Alaei, Y. Kinoshita, C. Bareille, R. Noguchi, M. Nakayama, S. Akebi, M. Sakano, K. Kawaguchi, M. Arita, S. Ideta, K. Tanaka, H. Kitazawa, K. Okazaki, M. Tokunaga, Y. Haga, S. Shin, H. S. Suzuki, R. Arita and T. Kondo, Nat Commun **11**, 2888/1-9 (2020).

6. *Observation and control of the weak topological insulator state in $ZrTe_5$: P. Zhang, R. Noguchi, K. Kuroda, C. Lin, K. Kawaguchi, K. Yaji, A. Harasawa, M. Lippmaa, S. Nie, H. Weng, V. Kandyba, A. Giampietri, A. Barinov, Q. Li, G. D. Gu, S. Shin and T. Kondo, Nat. Commun. **12**, 406 (2021).

Matsunaga group

We have investigated light-matter interactions and light-induced nonequilibrium phenomena in solids by utilizing terahertz (THz) pulse. We have studied nonlinear THz responses and nonequilibrium dynamics of carries in Dirac and Weyl semimetals. We have also developed optical parametric amplification of low-frequency infrared pulses in the intermediate region between THz frequency and mid-infrared, *167*., from 16.9 to 44.8 THz (6.7–17.8 μm) based on the intra-pulse differential frequency generation in GaSe. The long-term phase drift of the THz-to-MIR pulses after two-stage OPA is as small as 16 mrad during a 6-h operation without any active feedback. Our scheme using the intra-pulse DFG and post-amplification proposes a new route to intense THz-to-MIR light sources with extreme phase stability.

1. *Efficient Terahertz Harmonic Generation with Coherent Acceleration of Electrons in the Dirac Semimetal Cd_3As_2: B. Cheng, N. Kanda, T. N. Ikeda, T. Matsuda, P. Xia, T. Schumann, S. Stemmer, J. Itatani, N. P. Armitage and R. Matsunaga, Phys. Rev. Lett. **124**, 117402 (2020).

2. *Room-temperature terahertz anomalous Hall effect in Weyl antiferromagnet Mn_3Sn thin films: T. Matsuda, N. Kanda, T. Higo, N. P. Armitage, S. Nakatsuji and R. Matsunaga, Nat Commun **11**, 909 (2020).

3. Opening a new route to multiport coherent XUV sources via intracavity high-order harmonic generation: N. Kanda, T. Imahoko, K. Yoshida, A. Tanabashi, A. Amani Eilanlou, Y. Nabekawa, T. Sumiyoshi, M. Kuwata-Gonokami and K. Midorikawa, Light: Sci. Appl. **9**, 168 (2020).

4. *Optical parametric amplification of phase-stable terahertz-to-mid-infrared pulses studied in the time domain: N. Kanda, N. Ishii, J. Itatani and R. Matsunaga, Optics Express **29**, 3479-3489 (2021).

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 academic year 2020, we have found that Bose–Einstein condensation (BEC) superconductivity is induced by disappearance of the nematic state in FeSe by high-resolution laser ARPES. In addition, we

† Joint research with outside partners.

have revealed a characteristic electron-phonon coupling during the photo-induced insulator-to-metal transition in Ta_2NiSe_5 by a newly developed analysis method, frequency-domain angle-resolved photoemission spectroscopy (FDARPES), based on the measurements of HHG laser time-resolved ARPES.

1. †*Photoinduced Phase Transition from Excitonic Insulator to Semimetal-like State in $Ta_2Ni_{1-x}Co_xSe_5$(x = 0.10): T. Mitsuoka, T. Suzuki, H. Takagi, N. Katayama, H. Sawa, M. Nohara, M. Watanabe, J. Xu, Q. Ren, M. Fujisawa, T. Kanai, J. Itatani, S. Shin, K. Okazaki and T. Mizokawa, J. Phys. Soc. Jpn. **89**, 124703 (2020).

2. Massive Suppression of Proximity Pairing in Topological $(Bi_{1-x}Sb_x)_2Te_3$ Films on Niobium: J. A. Hlevyack, S. Najafzadeh, M. -K. Lin, T. Hashimoto, T. Nagashima, A. Tsuzuki, A. Fukushima, C. Bareille, Y. Bai, P. Chen, R. -Y. Liu, Y. Li, D. Fl"ototto, J. Avila, J. N. Eckstein, S. Shin, K. Okazaki and T. -C. Chiang, Phys. Rev. Lett. **124**, 236402 (2020).

3. Bose-Einstein condensation superconductivity induced by disappearance of the nematic state: T. Hashimoto, Y. Ota, A. Tsuzuki, T. Nagashima, A. Fukushima, S. Kasahara, Y. Matsuda, K. Matsuura, Y. Mizukami, T. Shibauchi, S. Shin and K. Okazaki, Sci. Adv. **6**, eabb9052 (2020).

4. *Devil's staircase transition of the electronic structures in CeSb: K. Kuroda, Y. Arai, N. Rezaei, S. Kunisada, S. Sakuragi, M. Alaei, Y. Kinoshita, C. Bareille, R. Noguchi, M. Nakayama, S. Akebi, M. Sakano, K. Kawaguchi, M. Arita, S. Ideta, K. Tanaka, H. Kitazawa, K. Okazaki, M. Tokunaga, Y. Haga, S. Shin, H. S. Suzuki, R. Arita and T. Kondo, Nat Commun **11**, 2888/1-9 (2020).

5. *Detecting electron-phonon coupling during photoinduced phase transition: T. Suzuki, Y. Shinohara, Y. Lu, M. Watanabe, J. Xu, K. L. Ishikawa, H. Takagi, M. Nohara, N. Katayama, H. Sawa, M. Fujisawa, T. Kanai, J. Itatani, T. Mizokawa, S. Shin and K. Okazaki, Phys. Rev. B **103**, L121105 (2021).

Kimura group

Kimura group started in July 2020, and our group works on developing new microscopic imaging technologies using advanced X-ray sources: X-ray free-electron lasers, synchrotron radiation, and high-order harmonics of ultrashort infrared laser pulses. In 2020, we developed a new X-ray microscopic imaging system at BL25SU of SPring-8 and BL1 of SACLA. We designed and fabricated novel X-ray optical components, such as focusing mirror and microfluidic device, by utilizing ultra-precision fabrication, measurement techniques, and semiconductor manufacturing processes.

1. Chi-Feng Huang, Wei-Hau Chang, Ting-Kuo Lee, Yasumasa Joti, Yoshinori Nishino, Takashi Kimura, Akihiro Suzuki, Yoshitaka Bessho, Tsung-Tse Lee, Mei-Chun Chen, Shun-Min Yang, Yeukuang Hwu, Shih-Hsin Huang, Po-Nan Li, Peilin Chen, Yung-Chieh Tseng, Che Ma, Tsui-Ling Hsu, Chi-Huey Wong, Kensuke Tono, Tetsuya Ishikawa, and Keng S. Liang: C.-F. Huang, W.-H. Chang, T.-K. Lee, Y. Joti, Y. Nishino, T. Kimura, A. Suzuki, Y. Bessho, T.-T. Lee, M.-C. Chen, S.-M. Yang, Y. Hwu, S.-H. Huang, P.-N. Li, P. Chen, Y.-C. Tseng, C. Ma, T.-L. Hsu, C.-H. Wong, K. Tono, T. Ishikawa and K. S. Liang, AIP Advances **10**, 055219 (2020).

2. Micro-liquid enclosure array and its semi-automated assembling system for x-ray free-electron laser diffractive imaging of samples in solution: T. Kimura, A. Suzuki, Y. Yang, Y. Niida, A. Nishioka, M. Takei, J. Wei, H. Mitomo, Y. Matsuo, K. Niikura, K. Ijiro, K. Tono, M. Yabashi, T. Ishikawa, T. Oshima, Y. Bessho, Y. Joti and Y. Nishino, Review of Scientific Instruments **91**, 083706 (2020).

3. A highly efficient nanofocusing system for soft x rays: Y. Takeo, H. Motoyama, T. Shimamura, T. Kimura, T. Kume, Y. Matsuzawa, T. Saito, Y. Imamura, H. Miyashita, K. Hiraguri, H. Hashizume, Y. Senba, H. Kishimoto, H. Ohashi and H. Mimura, Applied Physics Letters **117**, 151104 (2020).

4. Design of two-stage soft-X-ray nano-focusing system with a ring-focusing mirror and quasi-Wolter mirror: Y. Takeo, H. Motoyama, T. Shimamura, T. Kimura, T. Kume, Y. Matsuzawa, T. Saito, Y. Imamura, H. Miyashita, K. Hiraguri, H. Hashizume, Y. Senba, H. Kishimoto, H. Ohashi and H. Mimura, in: *PROCEEDINGS OF SPIE* (SPIE, 2020), 114920N.

5. Design of ultrashort Kirkpatrick-Baez mirror for soft x-ray nanofocusing: T. Shimamura, Y. Takeo, T. Kimura, H. Hashizume, Y. Senba, H. Kishimoto, H. Ohashi and H. Mimura, in: *PROCEEDINGS OF SPIE* (SPIE, 2020), 114920P.

* Joint research among groups within ISSP.

The Institute for Solid State Physics (ISSP), The University of Tokyo

Address	5-1-5 Kashiwanoha, Kashiwa, Chiba, 277-8581, Japan
Phone	+81-4-7136-3207
Home Page	https://www.issp.u-tokyo.ac.jp