Publications (2021.1 - 2022.4)

Division of Condensed Matter Science

Mori group

We have successfully developed and unveiled unprecedented functional properties for the molecular materials and systems. The major achievements in 2021 are (1) to develop the simplest model for doped PEDOT (Poly(3,4-ethylenedioxythiophene)), single-crystalline EDOT dimer radical cation salts, (2) to investigate effects of mechanical grinding on the phase behavior and anhydrous proton conductivity of imidazolium hydrogen succinate, and (3) to investigate modulation of the electronic states and magnetic properties of Nickel catecholdithiolene complex by oxidation-coupled deprotonation.

1. †Effects of mechanical grinding on the phase behavior and anhydrous proton conductivity of imidazolium hydrogen succinate: S. Dekura, Y. Sunairi, K. Okamoto, F. Takeiri, G. Kobayashi, Y. Hori, Y. Shigeta and H. Mori, Solid State Ionics **372**, 115775 (2021).

2. †Proton Conduction Mechanism for Anhydrous Imidazolium Hydrogen Succinate Based on Local Structures and Molecular Dynamics: Y. Hori, S. Dekura, Y. Sunairi, T. Ida, M. Mizuno, H. Mori and Y. Shigeta, J. Phys. Chem. Lett. **12**, 5390 (2021).

3. * 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).

4. 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).

5. 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).

6. *Ferromagnetism out of charge fluctuation of strongly correlated electrons in κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Br: M. Yamashita, S. Sugiura, A. Ueda, S. Dekura, T. Terashima, S. Uji, Y. Sunairi, H. Mori, E. I. Zhilyaeva, S. A. Torunova, R. N. Lyubovskaya, N. Drichko and C. Hotta, npj Quantum Mater. **6**, 87 (2021).

7. *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).

8. 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 **9**, 10718-10726 (2021).

9. †Magnetic and Structural Properties of Organic Radicals Based on Thienyl- and Furyl-Substituted Nitronyl Nitroxide: T. Sugano, S. J. Blundell, W. Hayes and H. Mori, Magnetochemistry **7**, 62 (2021).

10. Conjugation length effect on the conducting behavior of single-crystalline oligo(3,4-ethylenedioxythiophene) (*n* EDOT) radical cation salts: R. Kameyama, T. Fujino, S. Dekura and H. Mori, Phys. Chem. Chem. Phys. **24**, 9130 (2022).

11. Proton–electron-coupled functionalities of conductivity, magnetism, and optical properties in molecular crystals: H. Mori, S. Yokomori, S. Dekura and A. Ueda, Chem. Commun., 10.1039.D1CC06826A (2022), in print.

12. 水素を使いこなすためのサイエンス　ハイドロジェノミクス : 森 初果 , (共立出版 , ISBN 978-4-320-04498-2, 2022).

Osada group

Two topological thermoelectric effects were investigated in the organic Dirac fermion system: (1) The nonlinear anomalous Ettingshausen effect (AEE) was predicted as a thermoelectric analogue of the nonlinear anomalous Hall effect (AHE) in the

* Joint research among groups within ISSP.

current-carrying state in two-dimensional (2D) massive Dirac fermion system. The thermoelectric Berry curvature dipole was introduced instead of the Berry curvature dipole. We estimated the possible nonlinear AEE in the weak charge ordering (CO) state in an organic conductor α-(BEDT-TTF)$_2$I$_3$, and found that it is in the observable range. (2) The quantized thermoelectric Hall effect (QTHE), which was theoretically proposed in the 2D massless Dirac fermion system at the high-magnetic-field quantum limit, was investigated in the real organic Dirac system α-(BEDT-TTF)$_2$I$_3$. The relatively large Zeeman splitting of the n=0 Landau level suppresses the QTHE causing the hump-like structure of Seebeck coefficient, which was observed in the experiment.

1. 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).

2. 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).

3. Thermoelectric Effect at Quantum Limit in Two-Dimensional Organic Dirac Fermion System with Zeeman Splitting: T. Osada, J. Phys. Soc. Jpn. **90**, 113703(1-4) (2021).

4. Observation of possible nonlinear anomalous Hall effect in organic two-dimensional Dirac fermion system: A. Kiswandhi and T. Osada, J. Phys.: Condens. Matter **34**, 105602(1-7) (2022).

5. Thermoelectric Hall Effect at High-Magnetic-Field Quantum Limit in Graphite as a Nodal-Line Semimetal: T. Osada, T. Ochi and T. Taen, J. Phys. Soc. Jpn. **91**, 063701(1-4) (2022).

6. 有機ディラック電子系におけるトポロジカル輸送現象：長田 俊人 , 固体物理 **57**, 227-240 (2022).

7. 有機ディラック電子系における非線形トポロジカル輸送現象： 長田 俊人 , キスワンディ アンディカ , 日本物理学会誌 **77**, 233-238 (2022).

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 resistivity measurements of YbRh$_2$Si$_2$, (2) thermal-Hall measurements of AFM skyrmions in MnSc$_2$S$_4$, (3) planar thermal Hall measurements of Kitaev candidate Na$_2$Co$_2$TeO$_6$, and (4) electric transports and NMR of EuIn$_2$As$_2$.

1. *Pressure-induced phase transition in the J_1-J_2 square lattice antiferromagnet RbMoOPO$_4$Cl: H. Takeda, T. Yamauchi, M. Takigawa, H. Ishikawa and Z. Hiroi, Phys. Rev. B **103**, 104406 (2021).

2. Tuning the Parity Mixing of Singlet-Septet Pairing in a Half-Heusler Superconductor: K. Ishihara, T. Takenaka, Y. Miao, Y. Mizukami, K. Hashimoto, M. Yamashita, M. Konczykowski, R. Masuki, M. Hirayama, T. Nomoto, R. Arita, O. Pavlosiuk, P. Wisniewski, D. Kaczorowski and T. Shibauchi, Phys. Rev. X **11**, 041048 (2021).

3. *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).

4. *Ferromagnetism out of charge fluctuation of strongly correlated electrons in κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Br: M. Yamashita, S. Sugiura, A. Ueda, S. Dekura, T. Terashima, S. Uji, Y. Sunairi, H. Mori, E. I. Zhilyaeva, S. A. Torunova, R. N. Lyubovskaya, N. Drichko and C. Hotta, npj Quantum Mater. **6**, 87 (2021).

5. * ヘリウムリサイクルへの取り組み－東京大学物性研究所の活動－: 勝本 信吾 , 鷺山 玲子 , 土屋 光 , 山下 穣 , 低温工学 **56**, 119 (2021).

6. Field-induced topological Hall effect in antiferromagnetic axion insulator candidate EuIn$_2$As$_2$: J. Yan, Z. Z. Jiang, R. C. Xiao, W. J. Lu, W. H. Song, X. B. Zhu, X. Luo, Y. P. Sun and M. Yamashita, Phys. Rev. Research **4**, 013163 (2022).

Division of Condensed Matter Theory

Tsunetsugu group

† Joint research with outside partners.

We have continued to study several topics of correlated electron systems and their nonequilibrium dynamics this year. One topic is the thermodynamics of a frustrated spin system, and we have studied the Kagome spin system with breathing lattice deformation. Mapping this system to an effective model of spin and chirality degrees of freedom, we have performed classical Monte Carlo simulations to investigate their thermodynamic properties. We have found a glassy behavior of chiralities, which may be understood as a nematic liquid. We have also continued a study of electric quadrupoles in the heavy fermion system. An analysis on the complex spatial structure of quadrupoles has been developed further to examine the effects of the cubic interactions characteristic to this system. As for the nonequilibrium issues, we have analyzed nonlinear optical responses of a Kitaev spin liquid and proposed their use for identifying such a liquid. We have also developed a WKB theory to study nonperturbative nonlinear optical effects. For statistical-mechanical aspects of periodically driven quantum systems, we have characterized the heating rate in isolated systems based on the Fermi golden rule. We have also developed a theory for determining nonequilibrium steady states in the systems subject to Markovian dissipation. In particular, a setup was proposed for realizing a time crystalline steady state accompanied by critical phenomena.

1. 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).

2. Nematicity Liquid in a Trimerized-Kagome Antiferromagnet: I. Tanaka and H. Tsunetsugu, J. Phys. Soc. Jpn. **90**, 063707 (2021).

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

4. Analytical WKB theory for high-harmonic generation and its application to massive Dirac electrons: H. Taya, M. Hongo and T. N. Ikeda, Phys. Rev. B **104**, L140305 (2021).

5. Fermi's golden rule for heating in strongly driven Floquet systems: T. N. Ikeda and A. Polkovnikov, Phys. Rev. B **104**, 134308 (2021).

6. 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).

7. Linear and nonlinear optical responses in Kitaev spin liquids: M. Kanega, T. N. Ikeda and M. Sato, Phys. Rev. Research **3**, L032024 (2021).

8. Nonequilibrium steady states in the Floquet-Lindblad systems: van Vleck's high-frequency expansion approach: T. N. Ikeda, K. Chinzei and M. Sato, SciPost Phys. Core **4**, 033 (2021).

9. Criticality and rigidity of dissipative discrete time crystals in solids: K. Chinzei and T. N. Ikeda, Phys. Rev. Research **4**, 023025 (2022).

10. 複数の秩序が生むドメイン壁の不安定性 -- 複合ドメイン壁の構造不安定性 --: 川原 光滋 , 常次 宏一 , 固体物理 **56**, 467-475 (2021).

11. ユニークな四極子秩序の安定化機構の発見 : 服部 一匡 , 石飛 尊之 , 常次 宏一 , 固体物理 **57**, 255-266 (2022).

Kato group

The main research subject of Kato Lab. is transport properties in mesoscopic and spintronic devices. We studied (1) heat transport via small quantum systems, (2) transmission properties of Josephson junction arrays, (3) spin pumping from ferromagnetic insulator to metallic systems, (4) many-body effect in multielectron quantum dot systems, (5) high-harmonic generation in semiconductors, (6) nonequilibrium transport through Kondo quantum dots, (7) nanorotors driven by the spin-rotation coupling, and (8) the fluctuation theorem in spin-Hall magnetoresistance.

1. Heat transport through a two-level system embedded between two harmonic resonators: T. Yamamoto and T. Kato, J. Phys.: Condens. Matter **33**, 395303(1-10) (2021).

2. *High-harmonic generation in GaAs beyond the perturbative regime: P. Xia, T. Tamaya, C. Kim, F. Lu, T. Kanai, N. Ishii, J. Itatani, H. Akiyama and T. Kato, Phys. Rev. B **104**, L121202(1-6) (2021).

3. Nonlinear Fermi liquid transport through a quantum dot in asymmetric tunnel junctions: K. Tsutsumi, Y. Teratani, R. Sakano and A. Oguri, Phys. Rev. B **104**, 235147(1-17) (2021).

4. Piezo-optic effect of high-harmonic generation in semiconductors: T. Tamaya and T. Kato, Phys. Rev. B **103**, 205202(1-10) (2021).

5. Spin current at a magnetic junction as a probe of the Kondo state: T. Yamamoto, T. Kato and M. Matsuo, Phys. Rev. B **104**, L121401(1-5) (2021).

* Joint research among groups within ISSP.

6. Spin pumping of two-dimensional electron gas with Rashba and Dresselhaus spin-orbit interactions: M. Yama, M. Tatsuno, T. Kato and M. Matsuo, Phys. Rev. B **104**, 054410(1-9) (2021).

7. Transmission of waves through a pinned elastic medium: T. Yamamoto, L. I. Glazman and M. Houzet, Phys. Rev. B **103**, 224211(1-17) (2021).

8. *Preparation and Readout of Multielectron High-Spin States in a Gate-Defined GaAs/AlGaAs Quantum Dot: H. Kiyama, K. Yoshimi, T. Kato, T. Nakajima, A. Oiwa and S. Tarucha, Phys. Rev. Lett. **127**, 086802(1-6) (2021).

9. Three-body correlations in nonlinear response of correlated quantum liquid: T. Hata, Y. Teratani, T. Arakawa, S. Lee, M. Ferrier, R. Deblock, R. Sakano, A. Oguri and K. Kobayashi, Nat. Commun. **12**, 3233(1-7) (2021).

10. †*DSQSS: Discrete Space Quantum Systems Solver: Y. Motoyama, K. Yoshimi, A. Masaki-Kato, T. Kato and N. Kawashima, Comput. Phys. Commun. **264**, 107944(1-9) (2021).

11. Kondo Effect and Phase Measurement in Double Quantum Dot in Parallel: Y. Zhang, R. Sakano and M. Eto, J. Phys. Soc. Jpn. **91**, 014703(1-10) (2022).

12. Current noise and Keldysh vertex function of an Anderson impurity in the Fermi-liquid regime: A. Oguri, Y. Teratani, K. Tsutsumi and R. Sakano, Phys. Rev. B **105**, 115409(1-37) (2022).

13. Einstein–de Haas Nanorotor: W. Izumida, R. Okuyama, K. Sato, T. Kato and M. Matsuo, Phys. Rev. Lett. **128**, 017701(1-6) (2022).

14. Fluctuation theorem for spin transport at insulating ferromagnetic junctions: T. Sato, M. Tatsuno, M. Matsuo and T. Kato, Journal of Magnetism and Magnetic Materials **546**, 168814(1-6) (2022).

15. 一歩進んだ理解を目指す物性物理学講義 : 加藤 岳生 , (サイエンス社 , 東京 , 2022).

Division of Nanoscale Science

Katsumoto group

A shot noise measurement system using a handmade HEMT and a preamplifier has been completed. Numerical simulation on the spin precession and division of electrons propagating on spin-resolved quantum Hall edge was carried out with the recursive Green function method. The simulation successfully reproduced the experimentally observed probability partition. Shot noise measurement was carried out on the flying spin qubit interferometer. We have found an anomalous decrease in the shot noise at higher bias, which has been explained by the approach of spin-resolved edge states.

1. Commensurability oscillations in the Hall resistance of unidirectional lateral superlattices: A. Endo, S. Katsumoto and Y. Iye, Phys. Rev. B **103**, 235303 (2021).

2. Homemade-HEMT-based transimpedance amplifier for high-resolution shot-noise measurements: T. Shimizu, M. Hashisaka, H. Bohuslavskyi, T. Akiho, N. Kumada, S. Katsumoto and K. Muraki, Review of Scientific Instruments **92**, 124712 (2021).

3. * ヘリウムリサイクルへの取り組み一東京大学物性研究所の活動一: 勝本 信吾 , 鷺山 玲子 , 土屋 光 , 山下 穣 , 低温工学 **56**, 119 (2021).

Otani group

This year, we focused on the topic related to the antiferromagnetic spintronics, namely the manipulation of the cluster magnetic octupole state in Mn_3X (X=Mn or Sn) thin films. Last year, we succeeded in the magnetic octupole state manipulation in Mn_3Sn by using spin-orbit torque. We further improved the readout voltage beyond 1 mV, a milestone for future applications for memory technology. Besides, we also demonstrated that the absence of shape anisotropy enables omnidirectional control and lifts the shape constraint in designing magnetic devices. Our international collaboration with Pohang University of Science and Technology in Korea and Peter Grünberg Institut in Germany on the novel spin-charge conversion study showed that the flow of orbital angular momentum plays a vital role in exerting nontrivial torque in ferromagnetic metal/Cu/Aluminum oxide trilayers. Another international collaboration on magnon-phonon coupling study with Huazhong University of Science and Technology demonstrated numerically that antiferromagnetic domain walls could oscillate at a relatively low frequency of the order of MHz. This finding is beneficial for antiferromagnetic devices, which require a stable antiferromagnetic domain wall velocity.

† Joint research with outside partners.

1. 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).

2. *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).

3. Influence of planar Hall effect on the output signal in a T-shaped spin conversion device: H. Mizuno, H. Isshiki, K. Kondou, Y. Zhu and Y. Otani, Appl. Phys. Lett. **119**, 092401 (2021).

4. *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 (2021).

5. *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).

6. 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).

7. *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).

8. 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).

9. *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).

10. *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).

11. Interaction between surface acoustic waves and spin waves in a ferromagnetic thin film: K. Yamamoto, M. Xu, J. Puebla, Y. Otani and S. Maekawa, Journal of Magnetism and Magnetic Materials **545**, 168672 (2022).

12. Efficient and controllable magnetization switching induced by intermixing-enhanced bulk spin–orbit torque in ferromagnetic multilayers: K. Zhang, L. Chen, Y. Zhang, B. Hong, Y. He, K. Lin, Z. Zhang, Z. Zheng, X. Feng, Y. Zhang, Y. Otani and W. Zhao, Applied Physics Reviews **9**, 011407 (2022).

Hasegawa group

We studied superconductivity of Pb atomic layers formed on vicinal substrates to investigate how surface steps with an interval shorter than the coherence length affect the two-dimensional superconductivity. Transport measurements revealed reduced critical temperature and enhanced critical magnetic field. Scanning tunneling microscopy (STM) exhibited elongated vortices along the steps. The oval-shaped vortices are Abrikosov-Josephson vortices squeezed in the direction perpendicular to the steps due to the reduced coherence length, which is also responsible for the enhanced critical fields. Our work demonstrates that vicinal substrates provide a unique platform to control macroscopic properties through the precise tuning of disorder. In collaboration with Prof. Bent Weber, Nanyang Univ., Singapore, we investigated heterostructures of a quantum spin Hall candidate *1T'*-WTe_2 grown by van der Waals epitaxy on superconductor $NbSe_2$ by STM. By analyzing the normal and superconducting density of states (DOS) by scanning probe spectroscopy across the interface, we found that strong hybridization of electronic states gives rise to a semimetallic DOS in the 2D bulk even in nominally band insulating crystals. Despite the strong hybridization, we found a measurable enhancement of the local DOS at the crystal edges in the normal state and a slight enhancement of the order parameter in the superconducting state.

1. 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).

2. †Reduction in magnetic coercivity of Co nanomagnets by Fe alloying: H.-H. Yang, C.-C. Hsu, K. Asakawa, W.-C. Lin and Y. Hasegawa, Nanoscale **13**, 16719-16725 (2021).

3. †Multiband superconductivity in strongly hybridized 1T'−WTe_2/$NbSe_2$ heterostructures: W. Tao, Z. J. Tong, A. Das, D.-Q. Ho, Y. Sato, M. Haze, J. Jia, Y. Que, F. Bussolotti, K. E. Johnson Goh, B. Wang, H. Lin, A. Bansil, S. Mukherjee, Y. Hasegawa and B. Weber, Phys. Rev. B **105**, 094512(1-14) (2022).

---

* Joint research among groups within ISSP.

4. Superconductivity near the saddle point in the two-dimensional Rashba system Si(111)−√3×√3−(Tl,Pb): T. Machida, Y. Yoshimura, T. Nakamura, Y. Kohsaka, T. Hanaguri, C. -R. Hsing, C. -M. Wei, Y. Hasegawa, S. Hasegawa and A. Takayama, Phys. Rev. B **105**, 064507(1-9) (2022).

5. Numerical simulations for ferromagnetic resonance of nano-size island structures probed by radio-frequency scanning tunneling microscopy: Y. Sato, M. Haze, H.-H. Yang, K. Asakawa, S. Takahashi and Y. Hasegawa, Jpn. J. Appl. Phys. **61**, 025001(1-6) (2022).

6. スパースモデリングを活用した走査トンネル顕微鏡像解析：土師 将裕，吉田 靖雄，長谷川 幸雄，表面と真空 **65**, 78-83 (2022).

7. 走査トンネル分光法：長谷川 幸雄，「図説表面分析ハンドブック」，日本表面真空学会，(朝倉出版，2021), 428-433.

Lippmaa group

We have worked on developing the pulsed laser deposition process. In particular, we have studied the effect of the high-energy ions in the ablation plume have on the properties of ceramic thin films. Our recent work shows that the plume energy is sufficient to cause local damage in thin films, as shown by thin film lattice parameter shifts from known bulk values. We have shown that the kinetic damage to thin films can be effectively reduced by introducing a light inert buffer gas into the process chamber. Deposition of films in the presence of high-pressure He ambient gas does not significantly reduce the deposition rate, but reduces the kinetic energy of the plume and thus enables the growth of higher-quality thin films with fewer point defects.

1. Nanopillar composite electrodes for solar-driven water splitting: M. Lippmaa, S. Kawasaki, R. Takahashi and T. Yamamoto, MRS Bulletin **46**, 142-151 (2021).

2. [†]He Buffer Gas for Moderating the Kinetic Energy of Pulsed Laser Deposition Plumes: R. Takahashi, T. Yamamoto and M. Lippmaa, Cryst. Growth Des. **21**, 5017-5026 (2021).

3. 単結晶薄膜の自立化プロセスの開発：高橋 竜太，リップマー ミック，セラミックス **56**, 451-454 (2021).

4. [*]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).

5. [†]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 2021: (1) The surface chemistry of hydrogen, formic acid and CO_2 on Cu(977), Pd-Cu(111) and Pd-Cu(997) surfaces was studied by SR-PES, IRAS, HREELS and TPD. (2) The adsorption/desorption of CH_4 on Pt(997) was studied by TPD, IRAS and SR-XPS. (3) The dry reforming of CH_4 with CO_2 on Pt(997) was studied by AP-XPS at SPring-8. (4) The reaction dynamics of CO + O -> CO_2 on Pt(111) was studied by van der Waals DFT calculations. (5) The micro-beam SR-XPS and AP-XPS were applied to study the MoS_2 edge in vacuum and under hydrogen pressure. (6) The narrow band and broad band THz pulse generation system has been newly constructed.

1. [†]Adsorption of CO_2 on Terrace, Step, and Defect Sites on Pt Surfaces: A Combined TPD, XPS, and DFT Study: Y. Wong, Y. H. Choi, S. Tanaka, H. Yoshioka, K. Mukai, H. H. Halim, A. R. Mohamed, K. Inagaki, Y. Hamamoto, I. Hamada, J. Yoshinobu and Y. Morikawa, J. Phys. Chem. C **125**, 23657 (2021).

2. [†*]Band Bending of n-GaN under Ambient H_2O Vapor Studied by X-ray Photoelectron Spectroscopy: Y. Imazeki, M. Sato, T. Takeda, M. Kobayashi, S. Yamamoto, I. Matsuda, J. Yoshinobu, M. Sugiyama and Y. Nakano, J. Phys. Chem. C **125**, 9011 (2021).

3. 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).

4. [†*]Comparative Study of H_2O and O_2 Adsorption on the GaN Surface: M. Sato, Y. Imazeki, T. Takeda, M. Kobayashi, S. Yamamoto, I. Matsuda, J. Yoshinobu, Y. Nakano and M. Sugiyama, J. Phys. Chem. C **125**, 25807 (2021).

[†] Joint research with outside partners.

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. 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).

7. Theoretical study on adsorption and reaction of polymeric formic acid on the Cu(111) surface: S. E. M. Putra, F. Muttaqien, Y. Hamamoto, K. Inagaki, A. Shiotari, J. Yoshinobu, Y. Morikawa and I. Hamada, Phys. Rev. Materials **5**, 075801 (2021).

8. †*Structure and electronic structure of van der Waals interfaces at a Au(1 1 1) 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).

9. †*Functionalization of the MoS_2 basal plane for activation of molecular hydrogen by Pd deposition: F. Ozaki, S. Tanaka, W. Osada, K. Mukai, M. Horio, T. Koitaya, S. Yamamoto, I. Matsuda and J. Yoshinobu, Applied Surface Science **593**, 153313 (2022).

10. †*Hydrogen absorption and diffusion behaviors in cube-shaped palladium nanoparticles revealed by ambient-pressure X-ray photoelectron spectroscopy: J. Tang, O. Seo, D. S. R. Rocabado, T. Koitaya, S. Yamamoto, Y. Nanba, C. Song, J. Kim, A. Yoshigoe, M. Koyama, S. Dekura, H. Kobayashi, H. Kitagawa, O. Sakata, I. Matsuda and J. Yoshinobu, Applied Surface Science **587**, 152797 (2022).

11. *Tracking Ultrafast Change of Multiterahertz Broadband Response Functions in a Photoexcited Dirac Semimetal Cd_3As_2 Thin Film: N. Kanda, Y. Murotani, T. Matsuda, M. Goyal, S. Salmani-Rezaie, J. Yoshinobu, S. Stemmer and R. Matsunaga, Nano Letters **22**, 2358 (2022).

12. ZrB_2(0001) 薄膜表面上の二次元 Ge 二重三角格子 : 深谷 有喜 , 吉信 淳 , アントワーヌ フロランス , 高村 (山田) 由紀子 , PF News **39-3**, 21-27 (2021).

13. 巻頭言　界面におけるエネルギー変換・輸送と現代の課題 : 吉信 淳 , 表面と真空 **64**, 539 (2021).

14. Hydrogenomics: Efficient and Selective Hydrogenation of Stable Molecules Utilizing Three Aspects of Hydrogen: K. Fukutani, J. Yoshinobu, M. Yamauchi, T. Shima and S. Orimo, Catal Lett **152**, 1583-1597 (2022).

15. 図説 表面分析ハンドブック : 日本表面真空学会 (編集), (朝倉書店 , 東京都 , 2021).

16. “水素 " を使いこなすためのサイエンス　ハイドロジェノミクス : 折茂 慎一 , 福谷 克之 , 藤田 健一（編）, (共立出版 , 東京都文京区 , 2022).

Akiyama group

In 2021, we fabricated new series of gain-switched 1030-1060nm InGaAs laser diodes (LDs) changing various device parameters and investigated stable short seed-pulse generation conditions below 10 ps by current injection. We started study on heat-recovery (HERC) solar cells, and photo-voltaic and thermo-electric hybrid tandem cells, in collaboration with AIST team. Collaborations on four-junction solar cells with China team and on CIGC cells with Tsukuba team have been started. As for bio- and chemical-physics, we had significant progress in time-resolved Raman spectroscopy on channel rhodopsin with semiconductor-laser-based light sources (collaboration between a D3 student Shibata-kun and Inoue-group). Good progress has been made in quantitative spectroscopy on bioluminescence quantum yield of new luciferin analogs (Akalumine, Tokeoni, etc.) and on photo-cleavage/photo-bleaching quantum yields of D-luciferin and coumarin-caged-luciferins, in collaboration with Gunma-university team.

1. *High-harmonic generation in GaAs beyond the perturbative regime: P. Xia, T. Tamaya, C. Kim, F. Lu, T. Kanai, N. Ishii, J. Itatani, H. Akiyama and T. Kato, Phys. Rev. B **104**, L121202(1-6) (2021).

2. *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).

3. Unidirectional output from a quantum-dot single-photon source hybrid integrated on silicon: R. Katsumi, Y. Ota, T. Tajiri, M. Kakuda, S. Iwamoto, H. Akiyama and Y. Arakawa, Opt. Express **29**, 37117 (2021).

4. 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).

* Joint research among groups within ISSP.

5. 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).

6. Reducing Shockley–Read–Hall recombination losses in the depletion region of a solar cell by using a wide-gap emitter layer: T. Nakamura, W. Yanwachirakul, M. Imaizumi, M. Sugiyama, H. Akiyama and Y. Okada, Journal of Applied Physics **130**, 153102 (2021).

7. Absorption Spectra for Firefly Bioluminescence Substrate Analog: TokeOni in Various pH Solutions: H. Ogawa, R. Ono, Y. Noguchi, N. Kitada, R. Saito-Moriya, S. A. Maki, H. Akiyama, H. Itabashi and M. Hiyama, Photochem Photobiol **97**, 1016 (2021).

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 **420**, 127660 (2021).

9. Electron–Hole Plasma Lasing Dynamics in $CsPbCl_m Br_{3-m}$ 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).

10. 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).

11. 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).

12. Diagnosing breakdown mechanisms in monocrystalline silicon solar cells via electroluminescence imaging: Y. Jia, Y. Wang, X. Hu, J. Xu, G. Weng, X. Luo, S. Chen, Z. Zhu and H. Akiyama, Solar Energy **225**, 463 (2021).

13. Improving the performance of Sb_2S_3 thin-film solar cells by optimization of VTD source-substrate proximity: R. Wang, Y. Wang, Y. Pan, D. Qin, G. Weng, X. Hu, J. Tao, X. Luo, S. Chen, Z. Zhu, J. Chu and H. Akiyama, Solar Energy **220**, 942 (2021).

14. Electroluminescence imaging of laser induced defect formation in $Cu(In, Ga)Se_2$ solar cell: Y. Jia, Y. Wang, X. Hu, G. Weng, J. Tian, X. Luo, S. Chen, Z. Zhu and H. Akiyama, Solar Energy Materials and Solar Cells **230**, 111160 (2021).

15. レーザー加工用 LD シード光源の開発―ピコ秒利得スイッチ半導体レーザー：中村 考宏 , 中前 秀一 , 金昌 秀 , ソダーバンル ハッサネット , 杉山 正和 , 秋山 英文 , レーザ加工学会誌 **28**, 30-35 (2021).

16. Subcells Analysis of Thin-Film Four-Junction Solar Cells Using Optoelectronic Reciprocity Relation: J. Long, Q. Sun, X. Li, P. Dai, M. Song, L. Zhu, H. Akiyama, J. Lu and S. Lu, Sol. RRL **5**, 2000542 (2021).

17. Photo-bleaching of firefly luciferin with UV irradiation: R. Kumagai, R. Ono, H. Akiyama, H. Itabashi and M. Hiyama, Chemical Physics Letters **792**, 139414 (2022).

18. Carrier dynamics of AlGaAs/AlAs asymmetric double quantum wells with different barrier thickness: Y. Liu, G. Weng, F. Cao, Y. Wang, W. Wan, C. Wang, H. Nakamae, C. Kim, X. Hu, X. Luo, S. Luo, S. Chen, J. Chu and H. Akiyama, Opt. Mater. Express **12**, 1291 (2022).

Sugino group

Target of Sugino group is to advance computational materials science using modern density functional theory (DFT). This was proceeded by improving the density functional through machine-learning of the many-body wave function of materials. Our machine-learning method was found to provide reasonably accurate electronic structures not only for molecules but also bulk solids, showing a promise for further improvement toward the chemical accuracy. Electron-phonon coupling is another key to the improvement. Effect of nuclear motion on the band gap was investigated using perturbative or non-perturbative method gaining insight into the material dependence. Applying DFT to various materials was intensively done for the phase problems of graphite intercalations, solid oxygen, and cuprates in addition to our continued study on electrochemical interfaces.

1. Optical representation of thermal nuclear fluctuation effect on band-gap renormalization: K. Ishii, J. Haruyama and O. Sugino, Phys. Rev. B **104**, 245144 (2021).

2. Functional-renormalization-group approach to classical liquids with short-range repulsion: A scheme without repulsive reference system: T. Yokota, J. Haruyama and O. Sugino, Phys. Rev. E **104**, 014124 (2021).

3. †Thermodynamic Analysis of Li-Intercalated Graphite by First-Principles Calculations with Vibrational and Configura-

† Joint research with outside partners.

tional Contributions: J. Haruyama, S. Takagi, K. Shimoda, I. Watanabe, K. Sodeyama, T. Ikeshoji and M. Otani, J. Phys. Chem. C **125**, 27891 (2021).

4. †*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).

5. †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, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **22**, 19401-19442 (2021).

6. †Machine-learning-based exchange correlation functional with physical asymptotic constraints: R. Nagai, R. Akashi and O. Sugino, Phys. Rev. Research **4**, 013106 (2022).

7. †Roadmap on Machine Learning in Electronic Structure: R. Nagai, R. Akashi and O. Sugino, Electron. Struct. **1**, 37-38 (2022).

Oka group

The Oka group has proposed a theory of geometric effects in non-adiabatic tunneling and applied it to strong field excitations in Dirac and Weyl semimetals.

1. Nonperturbative topological current in Weyl and Dirac semimetals in laser fields: R. M. A. Dantas, Z. Wang, P. Surówka and T. Oka, Phys. Rev. B **103**, L201105 (2021).

2. 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).

3. Nonadiabatic nonlinear optics and quantum geometry — Application to the twisted Schwinger effect: S. Takayoshi, J. Wu and T. Oka, SciPost Phys. **11**, 075 (2021).

Inoue group

In 2021, we reported a new machine learning method to predict rhodopsin genes having red-shifted absorption. By applying this method, ion pumping rhodopsin exhibiting absorption wavelength 40-nm longer than known proteins was discovered. The crystal structure of schizorhodopsin (SzR), which is a new type of inward proton pump first characterized in 2020, by X-ray crystallography. It revealed that transmembrane helices of SzR are shortened on the cytoplasmic side enabling rapid proton release to the cytoplasmic solvent. We found thermostable SzRs from thermophilic archaea. This finding suggests that in addition to general outward proton pumping rhodopsins, various types of microbial rhodopsins are used in high-temperature environments.

1. 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 **60**, 899-907 (2021).

2. 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).

3. Thermostable light-driven inward proton pump rhodopsins: Y. Kawasaki, M. Konno and K. Inoue, Chemical Physics Letters **779**, 138868 (2021).

4. 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).

5. Pro219 is an electrostatic color determinant in the light-driven sodium pump KR2: Y. Nakajima, L. Pedraza-González, L. Barneschi, K. Inoue, M. Olivucci and H. Kandori, Commun. Biol. **4**, 1185 (2021).

6. Ion Transport Activity Assay for Microbial Rhodopsin Expressed in Escherichia coli Cells: M. Konno, K. Inoue and H. Kandori, bio-protocol **11**, e4115 (2021).

7. Heliorhodopsin Evolution Is Driven by Photosensory Promiscuity in Monoderms: P.-A. Bulzu, V. S. Kavagutti, M.-C. Chiriac, C. D. Vavourakis, K. Inoue, H. Kandori, A.-S. Andrei, R. Ghai and S. J. Hallam, mSphere **6**, e00661-21 (2021).

8. Structural characterization of proton-pumping rhodopsin lacking a cytoplasmic proton donor residue by X-ray crystallography: K. Suzuki, M. D. C. Marín, M. Konno, R. Bagherzadeh, T. Murata and K. Inoue, J. Biol. Chem. **298**, 101722 (2022).

---

* Joint research among groups within ISSP.

9. Diverse heliorhodopsins detected via functional metagenomics in freshwater *Actinobacteria* , *Chloroflexi* and *Archaea*: A. Chazan, A. Rozenberg, K. Mannen, T. Nagata, R. Tahan, S. Yaish, S. Larom, K. Inoue, O. Béjà and A. Pushkarev, Environmental Microbiology **24**, 110-121 (2022).

10. Saccharibacteria harness light energy using type-1 rhodopsins that may rely on retinal sourced from microbial hosts: A. L. Jaffe, M. Konno, Y. Kawasaki, C. Kataoka, O. Béjà, H. Kandori, K. Inoue and J. F. Banfield, ISME J, published on the web (2022).

11. 第３のロドプシン：ヘリオロドプシン：井上 圭一 , 化学と工業 **74**, 307 (2021).

12. Expanding horizons of biosciences by light-control: M. Kataoka and T. Nagata, Biophysics and Physicobiology **18**, 13-15 (2021).

13. Microbial Rhodopsins: The Last Two Decades: A. Rozenberg, K. Inoue, H. Kandori and O. Béjà, Annu. Rev. Microbiol. **75**, published on the web (2021).

14. Rhodopsins at a glance: T. Nagata and K. Inoue, J. Cell Sci. **134**, jcs258989 (2021).

15. 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.

16. 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.

17. 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 continued theoretical studies on a wide range of subjects in many-body physics. In particular, we successfully implemented the "Level Spectroscopy" based on tensor-network renormalization group on the 2-dimensional classical XY model. This model is a canonical model to exhibit the Berezinskii-Kosterlitz-Thouless (BKT) transition, which is a prototypical topological phase transition. Although it has been studied for more than half century, the logarithmic correction makes a precise determination of the transition point rather challenging. By utilizing the powerful finite-scaling of conformal field theory and the modern numerical algorithm, we have succeeded in an extremely accurate determination of the BKT transition point, as well as a visualization of the Renormalization-Group flow based on the actual numerical data.

1. Resolving the Berezinskii-Kosterlitz-Thouless transition in the two-dimensional XY model with tensor-network-based level spectroscopy: A. Ueda and M. Oshikawa, Phys. Rev. B **104**, 165132 (2021).

2. †SU(4)-symmetric quantum spin-orbital liquids on various lattices: M. G. Yamada, M. Oshikawa and G. Jackeli, Phys. Rev. B **104**, 224436 (2021).

3. †Two-wire junction of inequivalent Tomonaga-Luttinger liquids: Y.-T. Kang, C.-Y. Lo, M. Oshikawa, Y.-J. Kao and P. Chen, Phys. Rev. B **104**, 235142 (2021).

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

5. Twisted Boundary Condition and Lieb-Schultz-Mattis Ingappability for Discrete Symmetries: Y. Yao and M. Oshikawa, Phys. Rev. Lett. **126**, 217201 (2021).

6. †Photon Echo from Lensing of Fractional Excitations in Tomonaga-Luttinger Spin Liquid: Z.-L. Li, M. Oshikawa and Y. Wan, Phys. Rev. X **11**, 031035 (2021).

7. Chiral approximation to twisted bilayer graphene: Exact intravalley inversion symmetry, nodal structure, and implications for higher magic angles: J. Wang, Y. Zheng, A. J. Millis and J. Cano, Phys. Rev. Research **3**,, 023155 (2021).

8. Topological field theories and symmetry protected topological phases with fusion category symmetries: K. Inamura, Journal of High Energy Physics **2021**, 204 (2021).

9. †Parafermionization, bosonization, and critical parafermionic theories: Y. Yao and A. Furusaki, J. High Energ. Phys.

† Joint research with outside partners.

2021, 285 (2021).

10. Fermionization and boundary states in 1+1 dimensions: Y. Fukusumi, Y. Tachikawa and Y. Zheng, SciPost Phys. **11**, 082 (2021).

11. †Remarks on compatibility between conformal symmetry and continuous higher-form symmetries: Y. Lee and Y. Zheng, Physical Review D **104**, 085005 (1-7) (2021).

12. Kramers-Wannier-like Duality Defects in (3+1)D Gauge Theories: J. Kaidi, K. Ohmori and Y. Zheng, Phys. Rev. Lett. **128**, 111601 (2022).

13. On lattice models of gapped phases with fusion category symmetries: K. Inamura, J. High Energ. Phys. **2022**, 36 (2022).

Nakatsuji group

A new era in quantum materials research arises, featuring discoveries of novel topological phases of matter and emergent quasi-particle 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. 6-GHz lattice response in a quantum spin-orbital liquid probed by time-resolved resonant x-ray scattering: K. Takubo, T. Mizokawa, H. Man, K. Yamamoto, Y. Zhang, Y. Hirata, H. Wadati, D. I. Khomskii and S. Nakatsuji, Phys. Rev. B **104**, 205110 (2021).

2. Logarithmic criticality in transverse thermoelectric conductivity of the ferromagnetic topological semimetal CoMnSb: H. Nakamura, S. Minami, T. Tomita, A. A. Nugroho and S. Nakatsuji, Phys. Rev. B **104**, L161114 (2021).

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

4. *Observation of spontaneous x-ray magnetic circular dichroism in a chiral antiferromagnet: S. Sakamoto, T. Higo, M. Shiga, K. Amemiya, S. Nakatsuji and S. Miwa, Phys. Rev. B **104**, 134431 (1-6) (2021).

5. *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).

6. Simultaneous enhancements of thermopower and electrical conductivity in quasi-one-dimensional α-$YbAlB_4$ single crystal: K. Kuga, M. Matsunami, S. Singh, S. Nakatsuji and T. Takeuchi, Appl. Phys. Lett. **119**, 223905 (2021).

7. トポロジカル磁性体が拓く新たな応用展開 量子制御による革新的機能の創製に向けて： 中辻 知，応用物理 **90**, 221-229 (2021).

8. * ワイル反強磁性金属 Mn_3Sn 薄膜の室温テラヘルツ異常ホール効果：松田 拓也，肥後 友也，神田 夏輝，松永 隆佑，応用物理 **90**, 752 (2021).

9. *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 (2021).

10. *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).

11. 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).

12. Monopolar and dipolar relaxation in spin ice $Ho_2Ti_2O_7$: Y. Wang, T. Reeder, Y. Karaki, J. Kindervater, T. Halloran, N. Maliszewskyi, Y. Qiu, J. A. Rodriguez, S. Gladchenko, S. M. Koohpayeh, S. Nakatsuji and C. Broholm, Science Advances **7**(1-10) (2021).

* Joint research among groups within ISSP.

13. Monopolar and dipolar relaxation in spin ice $Ho_2Ti_2O_7$: Y. Wang, T. Reeder, Y. Karaki, J. Kindervater, T. Halloran, N. Maliszewskyj, Y. Qiu, J. A. Rodriguez, S. Gladchenko, S. M. Koohpayeh, S. Nakatsuji and C. Broholm, Sci. Adv. **7**, eabg0908 (2021).

14. *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).

15. Spin-orbital liquid in $Ba_3CuSb_2O_9$ stabilized by oxygen holes: K. Takubo, H. Man, S. Nakatsuji, K. Yamamoto, Y. Zhang, Y. Hirata, H. Wadati, A. Yasui, T. Mizokawa and D. I. Khomskii, Phys. Rev. Materials **5**, 075002 (2021).

16. Giant field-like torque by the out-of-plane magnetic spin Hall effect in a topological antiferromagnet: K. Kondou, H. Chen, T. Tomita, M. Ikhlas, T. Higo, A. H. MacDonald, S. Nakatsuji and Y. Otani, Nat Commun **12**, 6491 (2021).

17. 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).

18. X-ray study of ferroic octupole order producing anomalous Hall effect: M. Kimata, N. Sasabe, K. Kurita, Y. Yamasaki, C. Tabata, Y. Yokoyama, Y. Kotani, M. Ikhlas, T. Tomita, K. Amemiya, H. Nojiri, S. Nakatsuji, T. Koretsune, H. Nakao, T.-H. Arima and T. Nakamura, Nat Commun **12**, 5582 (2021).

19. High-temperature antiferromagnetism in Yb based heavy fermion systems proximate to a Kondo insulator: S. Suzuki, K. Takubo, K. Kuga, W. Higemoto, T. U. Ito, T. Tomita, Y. Shimura, Y. Matsumoto, C. Bareille, H. Wadati, S. Shin and S. Nakatsuji, Phys. Rev. Research **3**, 023140 (2021).

20. *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).

21. *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).

22. Logarithmic Criticality in Transverse Thermoelectric Conductivity of the Ferromagnetic Topological Semimetal CoMnSb: H. Nakamura, S. Minani, T. Tomita, A. A. Nugroho and S. Nakatsuji, Condensed Materials Materials Science arXiv:2105.12098, 1-6 (2021).

23. Phonon spectrum of $Pr_2Zr_2O_7$ and $Pr_2Ir_2O_7$ as evidence of coupling of the lattice with electronic and magnetic degrees of freedom: Y. Xu, H. Man, N. Tang, T. Ohtsuki, S. Baidya, S. Nakatsuji, D. Vanderbilt and N. Drichko, Phys. Rev. B **105**, 075137 (2022).

24. Ferrimagnetic compensation and its thickness dependence in TbFeCo alloy thin films: M. Ishibashi, K. Yakushiji, M. Kawaguchi, A. Tsukamoto, S. Nakatsuji and M. Hayashi, Applied Physics Letters **120**, 022405-1 and 4 (2022).

25. Topological Magnets: Functions Based on Berry Phase and Multipoles: S. Nakatsuji and R. Arita, Annu. Rev. Condens. Matter Phys. **13**, annurev-conmatphys-031620-103859 (2022).

Miwa group

We have studied the following topics this year: (1) Time-resolved spin dynamics and (2) x-ray magnetic circular dichroism on a chiral antiferromagnet Mn_3Sn, (3) microscopic understanding of perpendicular magnetic anisotropy at Fe/MgO. In topic (1), we find giant effective damping of the octupole polarization (ferroic order in the chiral antiferromagnet Mn_3Sn) due to exchange enhanced spin dynamics (Small Sci. **1**, 2000062). This is a work in collaboration with Nakatsuji and Otani groups. In topic (2), we have succeeded in preparing an epitaxial thin film of Mn_3Sn(1-100) and observing x-ray magnetic circular dichroism signals from the octupole polarization in Mn_3Sn. The signal comes from the magnetic dipole Tz term of Mn atoms (Phys. Rev. B **104**, 134431). This is a work in collaboration with Nakatsuji group. In topic (3), we find the perpendicular magnetic anisotropy in Fe/MgO system can be enhanced by reducing in-plane tensile strain in Fe ultrathin film (Phys. Rev. B **104**, L140406).

1. Influence of epitaxial strain on the perpendicular magnetic anisotropy of Fe/MgO systems: M. Shiga, S. Sakamoto, T. Tsujikawa, R. Ando, K. Amemiya and S. Miwa, Phys. Rev. B **104**, L140406 (1-6) (2021).

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

3. *Observation of spontaneous x-ray magnetic circular dichroism in a chiral antiferromagnet: S. Sakamoto, T. Higo, M.

† Joint research with outside partners.

Shiga, K. Amemiya, S. Nakatsuji and S. Miwa, Phys. Rev. B **104**, 134431 (1-6) (2021).

4. Quasi-maser operation using magnetic tunnel junctions: Y. Yamada, M. Goto, T. Yamane, N. Degawa, T. Suzuki, A. Shimura, S. Aoki, T. Mizuno, J. Urabe, S. Hara, S. Miwa and Y. Suzuki, Appl. Phys. Lett. **118**, 192402 (1-5) (2021).
5. 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).
6. *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).
7. *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).
8. Investigation of the thermal tolerance of 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, Sci Rep **11**, 10583 (2021).
9. *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).
10. *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).
11. Synthetic Rashba spin–orbit system using a silicon metal-oxide semiconductor: S. Lee, H. Koike, M. Goto, S. Miwa, Y. Suzuki, N. Yamashita, R. Ohshima, E. Shigematsu, Y. Ando and M. Shiraishi, Nat. Mater. **20**, 1228-1232 (2021).
12. Reservoir computing based on spintronics technology (p339-p360), Reservoir computing [Editor: K. Nakajima and I. Fischer]: T. Taniguchi, S. Tsunegi, S. Miwa, K. Fujii, H. Kubota and K. Nakajima, (Springer, Singapore, 2021).
13. Electron Correlation Enhances Orbital Polarization at a Ferromagnetic Metal/Insulator Interface: Depth-Resolved X-ray Magnetic Circular Dichroism and First-Principles Study: S. Sakamoto, M. Tsujikawa, M. Shirai, K. Amemiya and S. Miwa, ACS Appl. Electron. Mater. **4**, 1794-1799 (2022).

Division of Data-Integrated Materials Science

Fukushima group

This year, we have developed a fundamental simulation code for investigating the material properties of permanent magnets and spintronic materials. The automatic exhaustive calculations, which are based on the all-electron full-potential (Korringa-Kohn-Rostoker) KKR Green's function method (FPKKR), have been performed. Since the potential is anisotropic rather than spherically symmetric, it is possible to calculate not only the magnetization and Curie temperature but also the magneto-crystalline anisotropy energy constant with high accuracy. The KKR Green's function method can be conveniently combined with the coherent potential approximation (CPA). It is free from using supercells, resulting in reduced computational costs drastically. Therefore, our code can perform efficient calculations for a huge number of compositions of disordered alloys, compared to the other simulation code. We have applied this code to several magnetic materials, such as YCo_5 alloys, $SmCo_5$ alloys, and $Sm_2Fe_{17}N_3$ alloys. We have also systematically investigated the electronic structure, intrinsic defect formation, and transport properties of Cu_2S by first-principles calculations, using a theoretical model called an acanthite-like structure. The transport properties of Cu_2S system have been successfully reproduced using an electron-phonon scattering method, highlighting the important role of relaxation time prediction in conductivity estimation instead of regarding it as a constant.

1. 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).
2. 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).
3. Ferromagnetism and giant magnetoresistance in zinc-blende FeAs monolayers embedded in semiconductor structures:

* Joint research among groups within ISSP.

L. D. Anh, T. Hayakawa, Y. Nakagawa, H. Shinya, T. Fukushima, M. Kobayashi, H. Katayama-Yoshida, Y. Iwasa and M. Tanaka, Nat. Commun. **12**, 4201(1-10) (2021).

4. 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).

5. 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 **23**, 9773-9784 (2021).

6. Low-temperature acanthite-like phase of Cu_2S: electronic and transport properties: H. N. Nam, K. Suzuki, T. Q. Nguyen, A. Masago, H. Shinya, T. Fukushima and K. Sato, Phys. Rev. B **105**, 075205(1-11) (2022).

7. A first-principles study on the electrical conductivity of $Ag_2S_{1-x}Se_x$ (x=0, 0.25, 0.5): Electron-phonon coupling: 71. H. N. Nam, K. Suzuki, A. Masago, T. Q. Nguyen, H. Shinya, T. Fukushima and K. Sato, Appl. Phys. Lett. **120**, 143903(1-6) (2022).

8. *Automatic exhaustive calculations of large material space by Korringa-Kohn-Rostoker coherent potential approximation method — Applied to equiatomic quaternary high entropy alloys: T. Fukushima, H. Akai, T. Chikyow and H. Kino, Pays. Rev. Mater. **6**, 023802(1-19) (2022).

9. Mn 基ホイスラー合金の磁気特性と電子状態：梅津 理恵 , 斉藤 耕太郎 , 小野 寛太 , 佐藤 和則 , 福島 鉄也 , 黒田 文彬 , 小口 多美夫 , まてりあ **60**, 205-211 (2021).

10. 半導体スピントロニクス材料のデザイン：佐藤 和則 , 真砂 啓 , 福島 鉄也 , 新屋ひ かり ,「スピントロニクスのための計算機ナノマテリアルデザイン」, 吉田博 , (内田老鶴圃 , 2022), 167-188.

Materials Design and Characterization Laboratory

Hiroi group

The high-pressure synthesis, crystal structure, and magnetic properties of four novel transition-metal oxyhydrides─$Ba_2NaVO_3H_3$, $Ba_2NaVO_{2.4}H_{3.6}$, $Ba_2NaCrO_{2.2}H_{3.8}$, and $Ba_2NaTiO_3H_3$─crystallizing in the double-perovskite structure were reported. We studied the pyrochlore oxide $Hg_2Os_2O_7$ through thermodynamic measurements, muon spin rotation (μSR) spectroscopy and neutron diffraction experiments. A magnetic transition, probably to an AIAO-type order, was observed at 88 K, while the resistivity showed a decrease at the transition and remained metallic down to 2 K. Thus, the ground state of $Hg_2Os_2O_7$ is most likely an AIAO semimetal, which is analogous to the intermediate-temperature state of $Cd_2Os_2O_7$. $Hg_2Os_2O_7$ exists on the verge of the metal–insulator boundary on the metal side and provides an excellent platform for studying the electronic instability of 5delectrons with moderate electron correlations and strong spin–orbit interactions. Substitution effects of Os for Ru in α-$RuCl_3$ are investigated in a wide composition range of $0 \leq x \leq 0.67$ in $Ru_{1-x}Os_xCl_3$ by X-ray and electron diffraction, magnetic susceptibility, heat capacity, and Raman spectroscopy measurements. Apart from the Kitaev physics with antiferromagnetic interactions increasing with x, a rich phase diagram is obtained, which includes an antiferromagnetic long-range order below 12 K for $x \leq 0.15$, a dome-shaped spin-singlet dimer phase below 130 K for $0.15 \leq x \leq 0.40$, and a magnetic short-range order for $x > 0.40$. NaAlSi is an sp electron superconductor crystallizing in a layered structure of the anti-PbFCl type with a relatively high transition temperature Tc of ~7 K. We successfully prepared single crystals of NaAlSi by a Na–Ga flux method and characterized their superconducting and normal-state properties through electrical resistivity, magnetization, and heat capacity measurements. A sharp superconducting transition with a Tc of 6.8 K is clearly observed, and heat capacity data suggest an anisotropic superconducting gap. Surprisingly, despite the sp electron system, the normal state is governed by the electron correlations, which is indicated by a T^2 resistivity and a Wilson ratio of 2.0. The origin of the electron correlation may be related to the orthogonal saddle-shaped Fermi surfaces derived from the Si px and py states, which intersect with the light Al s bands to form the nodal lines near the Fermi level.

1. Extremely Large Magnetoresistance in the Hourglass Dirac Loop Chain Metal β-ReO2: D. Hirai, T. Anbai, S. Uji, T. Oguchi and Z. Hiroi, J. Phys. Soc. Jpn. **90**, 094708 (2021).

2. Superconductivity in the Topological Nodal-line Semimetal NaAlSi: T. Yamada, D. Hirai, H. Yamane and Z. Hiroi, J. Phys. Soc. Jpn. **90**, 034710 (2021).

3. *Universal Dynamics of Magnetic Monopoles in Two-Dimensional Kagomé Ice: H. Takatsu, K. Goto, T. J. Sato, J. W. Lynn, K. Matsubayashi, Y. Uwatoko, R. Higashinaka, K. Matsuhira, Z. Hiroi and H. Kadowaki, J. Phys. Soc. Jpn. **90**, 123705(1-4) (2021).

† Joint research with outside partners.

4. *Phase transition in the 5d(1) double perovskite Ba_2CaReO_6 induced by high magnetic field: H. Ishikawa, D. Hirai, A. Ikeda, M. Gen, T. Yajima, A. Matsuo, Y. H. Matsuda, Z. Hiroi and K. Kindo, Phys. Rev. B **104**, 174422(7) (2021).

5. *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).

6. †*Quantum antiferromagnet bluebellite comprising a maple-leaf lattice made of spin-1/2 Cu^{2+} ions: Y. Haraguchi, A. Matsuo, K. Kindo and Z. Hiroi, Phys. Rev. B **104**, 174439(6) (2021).

7. *Dimensional reduction by geometrical frustration in a cubic antiferromagnet composed of tetrahedral clusters: R. Okuma, M. Kofu, S. Asai, M. Avdeev, A. Koda, H. Okabe, M. Hiraishi, S. Takeshita, K. M. Kojima, R. Kadono, T. Masuda, K. Nakajima and Z. Hiroi, Nat. Commun. **12**, 4382(1-7) (2021).

8. Modern Alchemy: Making “Plastics” from Paper: Y. Iwamiya, M. Kawai, D. Nishio-Hamane, M. Shibayama and Z. Hiroi, Ind. Eng. Chem. Res. **60**, 355 (2021).

9. Pyrochlore oxide $Hg_2Os_2O_7$ on verge of metal–insulator boundary: K. Kataoka, D. Hirai, A. Koda, R. Kadono, T. Honda and Z. Hiroi, J. Phys.: Condens. Matter **34**, 135602 (2022).

10. Dimer Crystallization Induced by Elemental Substitution in the Honeycomb Lattice of $Ru_{1-x}Os_xCl_3$: K. Kataoka, D. Wulferding, T. Yajima, D. Nishio-Hamane, D. Hirai, S. Lee, K.-Y. Choi and Z. Hiroi, J. Phys. Soc. Jpn. **91**, 014801 (2022).

11. Unusual Resistive Transitions in the Nodal-Line Semimetallic Superconductor NaAlSi: D. Hirai, T. Ikenobe, T. Yamada, H. Yamane and Z. Hiroi, J. Phys. Soc. Jpn. **91**, 024702 (2022).

12. Electronic states of metallic electric toroidal quadrupole order in $Cd_2Re_2O_7$ determined by combining quantum oscillations and electronic structure calculations: H. T. Hirose, T. Terashima, D. Hirai, Y. Matsubayashi, N. Kikugawa, D. Graf, K. Sugii, S. Sugiura, Z. Hiroi and S. Uji, Phys. Rev. B **105**, 035116 (2022).

13. High-Pressure Synthesis of Transition-Metal Oxyhydrides with Double-Perovskite Structures: T. Yajima, K. Takahashi, H. Nakajima, T. Honda, K. Ikeda, T. Otomo and Z. Hiroi, Inorg. Chem. **61**, 2010 (2022).

14. Surface Functionalization of Non-Woven Fabrics Using a Novel Silica-Resin Coating Technology: Antiviral Treatment of Non-Woven Fabric Filters in Surgical Masks: C. Tsutsumi-Arai, Y. Iwamiya, R. Hoshino, C. Terada-Ito, S. Sejima, K. Akutsu-Suyama, M. Shibayama, Z. Hiroi, R. Tokuyama-Toda, R. Iwamiya, K. Ijichi, T. Chiba and K. Satomura, IJERPH **19**, 3639 (2022).

Kawashima group

We developed efficient methods, algorithms, parallelized programs, and sometimes new concepts, based on novel numerical techniques including the tensor network (TN) method and applied them to relevant physical problems. To list subjects of our research in 2021, (1) Development of new TN methods [Morita, PRB103][Tu, PRB103], (2) TN study of surface critical phenomena [Fukusumi, PRB104][Iino, JSP182], (3) Study of TN ground states such as Kitaev spin liquid [Lee, PRB104][Katsura, PRR3], (4) Study of spin liquid in frustrated spin systems [Ogino, PRB103 & PRB104][Kohshiro, PRB104], (5) TN implementation of rael-space renormalization group [Lyu, PRR3], (6) Development of open-source applications [Motoyama, CPC264][Hoshi, CPC258], (7) Application of data-scientific techniques to materials science [Harashima, PRM5]

1. 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).

2. Anisotropy as a diagnostic test for distinct tensor-network wave functions of integer- and half-integer-spin Kitaev quantum spin liquids: H.-Y. Lee, T. Suzuki, Y. B. Kim and N. Kawashima, Phys. Rev. B **104**, 024417(1-13) (2021).

3. 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).

4. Generating function for tensor network diagrammatic summation: W.-L. Tu, H.-K. Wu, N. Schuch, N. Kawashima and J.-Y. Chen, Phys. Rev. B **103**, 205155 (2021).

5. Global optimization of tensor renormalization group using the corner transfer matrix: S. Morita and N. Kawashima, Phys. Rev. B **103**, 045131(1-6) (2021).

6. Multiple magnetization plateaus induced by farther neighbor interactions in an S=1 two-leg Heisenberg spin ladder: H. Kohshiro, R. Kaneko, S. Morita, H. Katsura and N. Kawashima, Phys. Rev. B **104**, 214409 (2021).

* Joint research among groups within ISSP.

7. Open spin chain realization of a topological defect in a one-dimensional Ising model: Boundary and bulk symmetry: Y. Fukusumi and S. Iino, Phys. Rev. B **104**, 125418 (2021).

8. Symmetry-protected topological phases and competing orders in a spin-1/2 XXZ ladder with a four-spin interaction: T. Ogino, S. Furukawa, R. Kaneko, S. Morita and N. Kawashima, Phys. Rev. B **104**, 075135 (2021).

9. †*DSQSS: Discrete Space Quantum Systems Solver: Y. Motoyama, K. Yoshimi, A. Masaki-Kato, T. Kato and N. Kawashima, Comput. Phys. Commun. **264**, 107944(1-9) (2021).

10. †*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).

11. "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).

12. Mott-insulator-like Bose-Einstein condensation in a tight-binding system of interacting bosons with a flat band: H. Katsura, N. Kawashima, S. Morita, A. Tanaka and H. Tasaki, Phys. Rev. Research **3**, 033190 (2021).

13. Scaling dimensions from linearized tensor renormalization group transformations: X. Lyu, R. G. Xu and N. Kawashima, Phys. Rev. Research **3**, 023048 (2021).

14. 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).

15. Energy Scale Deformation on Regular Polyhedra: T. Eguchi, S. Oga, H. Katsura, A. Gendiar and T. Nishino, J. Phys. Soc. Jpn. **91**, 034001 (2022).

16. Universal and non-universal correction terms of Bose gases in dilute region: a quantum Monte Carlo study: A. Masaki-Kato, Y. Motoyama and N. Kawashima, J. Phys. Soc. Jpn. **90**, 034711(1-8) (2022).

17. *Unconventional dual 1D–2D quantum spin liquid revealed by ab initio studies on organic solids family: K. Ido, K. Yoshimi, T. Misawa and M. Imada, npj Quantum Mater. **7**, 48 (2022).

18. Cartesian Operator Factorization Method for Hydrogen: X. Lyu, C. Daniel and J. K. Freericks, Atoms **10**, 14 (2022).

Uwatoko group

The transport and optical properties of Ta_2NiSe_5 have been measured under high pressures up to ~ 9 GPa and present the complete phase diagram of the high-pressure semi-metallic phase above P_s ~ 3 GPa. Also, we discovered bulk superconductivity with transition temperature T_{sc} up to 1.2 K only around P_c, which further justifies the strong electron–lattice coupling. We study the interplay between CDW and SC in CsV_3Sb_5 via measurements of resistivity, dc and ac magnetic susceptibility under various pressures up to 6.6 GPa. The CDW transition decreases with pressure and experiences a subtle modification at $P_{c1} \approx 0.6$–0.9 GPa before it vanishes entirely at $P_{c2} \approx 2$ GPa. We study the electronic and magnetic properties of $CrGeTe_3$ single crystals by varying pressure up to 11.0 GPa using dc magnetic susceptibility and resistivity measurement. We demonstrate that pressure can be used as a suitable parameter to control both magnetic and electrical properties of $CrGeTe_3$ by tuning the charge transfer energy gap between the Te-p valence band and the Cr-e_g conduction band. Moreover, the lack of concurrent structural transition and spin crossover across the insulator-metal transition (IMT) makes $CrGeTe_3$ a unique vandal van der Waals material and provides a novel example of bandwidth-controlled IMT. We have systematically investigated superconductivity in Bi single crystal up to 6.2 GPa. These unusual regular state transport and superconducting properties suggest a possible unconventional superconductivity scenario for the Bi-III phase. We have investigated the external pressure effect on the resistance and the ARPES on $BiSbTe_3$. It is observed that with an increase of pressure, resistance decreases and at a value of 8 GPa a sharp drop in resistance is observed which indicates the occurrence of superconductivity. With further pressure increase, the superconducting transition temperature (T_c) increases and at 14 GPa it shows the maximum T_c (~ 3.3 K). This may indicate that the superconducting transition might be due to the change in the bulk band structure in $BiSbTe_3$. The theoretical study suggests that surface states remain topologically protected and bulk band structure changes under applied pressure.

1. Hybridization-Gap Formation and Superconductivity in the Pressure-Induced Semimetallic Phase of the Excitonic Insulator Ta_2NiSe_5: K. Matsubayashi, H. Okamura, T. Mizokawa, N. Katayama, A. Nakano, H. Sawa, T. Kaneko, T. Toriyama, T. Konishi, Y. Ohta, H. Arima, R. Yamanaka, A. Hisada, T. Okada, Y. Ikemoto, T. Moriwaki, K. Munakata, A. Nakao, M. Nohara, Y. Lu, H. Takagi and Y. Uwatoko, J. Phys. Soc. Jpn. **90**, 074706(1-6) (2021).

2. *Universal Dynamics of Magnetic Monopoles in Two-Dimensional Kagomé Ice: H. Takatsu, K. Goto, T. J. Sato, J. W.

† Joint research with outside partners.

Lynn, K. Matsubayashi, Y. Uwatoko, R. Higashinaka, K. Matsuhira, Z. Hiroi and H. Kadowaki, J. Phys. Soc. Jpn. **90**, 123705(1-4) (2021).

3. 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).

4. Effects of disorder and hydrostatic pressure on charge density wave and superconductivity in 2*H*-TaS_2: S. Xu, J. Gao, Z. Liu, K. Chen, P. Yang, S. Tian, C. Gong, J. Sun, M. Xue, J. Gouchi, X. Luo, Y. Sun, Y. Uwatoko, H. Lei, B. Wang and J. Cheng, Phys. Rev. B **103**, 224509(1-8) (2021).

5. High-pressure insulating phase of Mo_4O_{11} with collapsed volume: Z. Y. Liu, P. F. Shan, K. Y. Chen, M. Marshall, S. Zhang, T. Yong, H. S. Deng, X. Yin, Y. Ding, H. M. Weng, Y. Uwatoko, P. Dera, W. Xie, Y. Sui and J. -G. Cheng, Phys. Rev. B **104**, 024105(1-10) (2021).

6. †Pressure-induced multicriticality and electronic instability in the quasi-kagome ferromagnet URhSn: A. Maurya, D. Bhoi, F. Honda, Y. Shimizu, A. Nakamura, Y. J. Sato, D. Li, Y. Homma, M. Sathiskumar, J. Gouchi, Y. Uwatoko and D. Aoki, Phys. Rev. B **104**, 195119(1-5) (2021).

7. Superconducting phase diagram and the evolution of electronic structure across charge density wave in underdoped 1T-$Cu_\delta TiSe_2$ under hydrostatic pressure: S. Xu, P. Yang, K. Chen, Z. Liu, W. Cui, Q. Hu, J. Sun, R. Ang, Y. Uwatoko, B. Wang and J. Cheng, Phys. Rev. B **104**, 134503(1-9) (2021).

8. Double Superconducting Dome and Triple Enhancement of *Tc* in the Kagome Superconductor CsV_3Sb_5 under High Pressure: K. Chen, N. Wang, Q. Yin, Y. Gu, K. Jiang, Z. Tu, C. Gong, Y. Uwatoko, J. Sun, H. Lei, J. Hu and J. -G. Cheng, Phys. Rev. Lett. **126**, 247001(1-8) (2021).

9. Nearly Room-Temperature Ferromagnetism in a Pressure-Induced Correlated Metallic State of the van der Waals Insulator $CrGeTe_3$: D. Bhoi, J. Gouchi, N. Hiraoka, Y. Zhang, N. Ogita, T. Hasegawa, K. Kitagawa, H. Takagi, K. H. Kim and Y. Uwatoko, Phys. Rev. Lett. **127**, 217203(1-7) (2021).

10. Abnormal transport properties of Bi-III superconducting phase in pressurized bismuth single crystal: Y. Zhang, J. Gouchi, K. Ishigaki, S. Nagasaki, Z. Shi and Y. Uwatoko, Supercond. Sci. Technol. **34**, 075009(1-7) (2021).

11. Discovery of Superconductivity in the Quasi-One-Dimensional $SrBi_2Se_4$ Single Crystals: Y. Zhang, X. Xing, Y. Meng, X. Yi, J. Gouchi, D. Bhoi, J. Feng, Y. Fan, W. Zhou, N. Zhou, Y. Uwatoko and Z. Shi, Chem. Mater. **33**, 6752-6760 (2021).

12. Observation of antiferromagnetic ordering from muon spin resonance study and the Kondo effect in a Dy-doped Bi_2Se_3 topological insulator: V. K. Gangwar, S. Kumar, M. Singh, P. Singh, L. Ghosh, D. Pal, P. Shahi, Y. Uwatoko, E. F. Schwier, K. Shimada, D. K. Sharma, S. Kumar and S. Chatterjee, J. Phys. D: Appl. Phys. **54**, 455302(1-10) (2021).

13. *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).

14. Pressure Dependence of Superconducting Properties, Pinning Mechanism, and Crystal Structure of the $Fe_{0.99}Mn_{0.01}Se_{0.5}Te_{0.5}$ Superconductor: K. Murugesan, G. Lingannan, K. Ishigaki, Y. Uwatoko, C. Sekine, Y. Kawamura, H. JunIchi, B. Joseph, P. Vajeeston, P. K. Maheswari, V. P. S. Awana and A. Sonachalam, ACS Omega **6**, 30419-30431 (2021).

15. †Author Correction: 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**, 1800 (2021).

16. Continuous control of classical-quantum crossover by external high pressure in the coupled chain compound $CsCuCl_3$: D. Yamamoto, T. Sakurai, R. Okuto, S. Okubo, H. Ohta, H. Tanaka and Y. Uwatoko, Nat Commun **12**, 4263(1-9) (2021).

17. †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).

18. †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).

19. Defect induced ferromagnetic ordering and room temperature negative magnetoresistance in MoTeP: D. Pal, S. Kumar,

* Joint research among groups within ISSP.

P. Shahi, S. Dan, A. Verma, V. K. Gangwar, M. Singh, S. Chakravarty, Y. Uwatoko, S. Saha, S. Patil and S. Chatterjee, Sci Rep **11**, 9104(1-9) (2021).

20. †Pressure-induced reconstitution of Fermi surfaces and spin fluctuations in S-substituted FeSe: T. Kuwayama, K. Matsuura, J. Gouchi, Y. Yamakawa, Y. Mizukami, S. Kasahara, Y. Matsuda, T. Shibauchi, H. Kontani, Y. Uwatoko and N. Fujiwara, Sci Rep **11**, 17265(1-7) (2021).

21. Quasi-one-dimensional superconductivity in the pressurized charge-density-wave conductor $HfTe_3$: Z. Y. Liu, J. Li, J. F. Zhang, J. Li, P. T. Yang, S. Zhang, G. F. Chen, Y. Uwatoko, H. X. Yang, Y. Sui, K. Liu and J. -G. Cheng, npj Quantum Mater. **6**, 90(1-12) (2021).

22. Competition between charge-density-wave and superconductivity in the kagome metal Rb_3Sb_5: N. N. Wang, K. Y. Chen, Q. W. Yin, Y. N. N. Ma, B. Y. Pan, X. Yang, X. Y. Ji, S. L. Wu, P. F. Shan, S. X. Xu, Z. J. Tu, C. S. Gong, G. T. Liu, G. Li, Y. Uwatoko, X. L. Dong, H. C. Lei, J. P. Sun and J. -G. Cheng, Phys. Rev. Research **3**, 043018(1-11) (2021).

23. Correlation of magnetocaloric effect through magnetic and electrical resistivity on Si doped Ni–Mn–In Heusler melt spun ribbon: P. Sivaprakash, S. Arumugam, S. Esakki Muthu, D. M. Raj Kumar, C. Saravanan, N. V. Rama Rao, Y. Uwatoko and R. Thiyagarajan, Intermetallics **137**, 107285(1-8) (2021).

24. 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).

25. 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).

26. Abrupt Change in Electronic States under Pressure in New Compound $EuPt_3Al_5$: T. Koizumi, F. Honda, Y. J. Sato, D. Li, D. Aoki, Y. Haga, J. Gouchi, S. Nagasaki, Y. Uwatoko, Y. Kaneko and Y. Ônuki, J. Phys. Soc. Jpn. **91**, 043704(1-5) (2022).

27. †Magnetization of Quaternary Heusler Alloy CoFeCrAl: S. Tsujikawa, I. Shigeta, J. Gouchi, T. Kanomata, R. Y. Umetsu, Y. Uwatoko and M. Hiroi, IEEE Trans. Magn. **58**, 1 (1-5) (2022).

28. †Sub-micrometer particle size effects on metastable phases for a photoswitchable Co–Fe Prussian blue analog: M. Itoi, I. Maurin, K. Boukheddaden, M. J. Andrus, D. R. Talham, E. Elkaim and Y. Uwatoko, Journal of Applied Physics **131**, 085110(1-11) (2022).

29. Pressure-driven superconducting dome in the vicinity of CDW in the pyrite-type superconductor CuS_2: L. F. Shi, Z. Y. Liu, J. Li, X. X. Zhang, N. N. Wang, Q. Cui, K. Y. Chen, Q. Y. Liu, P. T. Yang, J. P. Sun, B. S. Wang, Y. Uwatoko, Y. Sui, H. X. Yang and J. -G. Cheng, Phys. Rev. Materials **6**, 014802(1-8) (2022).

30. Temperature-Pressure Phase Diagram and Possible Pressure-Driven New Electronic Phase in the Polar Metal $LiOsO_3$: J. -G. Cheng, J. -S. Zhou and Y. Uwatoko, ECS J. Solid State Sci. Technol. **11**, 023008(1-4) (2022).

Ozaki group

To discover novel materials having unknown structures, we performed high-throughput calculations for structural exploration based on computational methods such as density functional theory (DFT) in two directions. One is to find densest binary and ternary sphere packing structures (DBSPs, DTSPs). The other is to find two dimensional compounds consisting of AB_2 composition. As the first issue, we addressed the DBSPs and DTSPs under periodic boundary conditions and present phase diagrams, including newly found 12 and 59 putative densest structures, respectively. To efficiently explore the DBSPs and DTSPs, we developed an unbiased random search approach based on both the piling-up method to generate initial structures in an unbiased way and the iterative balance method to optimize the volume of a unit cell while keeping the overlap of hard spheres minimized. It turned out that many of DBSPs and DTSPs correspond to real crystals, suggesting that the diverse structures of DBSPs and DTSPs can be effectively used as structural prototypes for searching ternary and quaternary crystal structures. As the second issue, we constructed a structure map for AB_2 type monolayers of 3844 compounds which are all the combinations of 62 elements selected from the periodic table. The structure map and its web version (http://www.openmx-square.org/2d-ab2/), which are obtained by symmetry-unconstrained geometry optimizations starting from ferromagnetic 1T, 1H and planar structures as the initial states, provide comprehensive structural trends of the 3844 compounds in two dimensional (2D) structures and correctly predict the structures of most of the existing 2D compounds such as transition metal dichalcogenides and MXenes having 1T or 1H type structures. Our structure map and database will promote efforts towards the synthesis of undiscovered 2D materials experimentally and investigating the properties of new structures theoretically.

† Joint research with outside partners.

1. Methods for constructing parameter-dependent flat-band lattices: T. Ogata, M. Kawamura and T. Ozaki, Phys. Rev. B **103**, 205119 (2021).

2. Scaling law for Rashba-type spin splitting in quantum-well films: R. Noguchi, K. Kuroda, M. Kawamura, K. Yaji, A. Harasawa, T. Iimori, S. Shin, F. Komori and T. Ozaki, Phys. Rev. B **104**, L180409 (2021).

3. The hidden competing phase revealed by first-principles calculations of phonon instability in the nearly optimally doped cuprate La1.875Sr0.125CuO4: C.-C. Lee, J.-Y. Chiu, Y. Yamada-Takamura and T. Ozaki, Phys. Rev. B **104**, 064114 (2021).

4. Densest ternary sphere packings: R. Koshoji and T. Ozaki, Phys. Rev. E **104**, 024101 (2021).

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

6. †*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).

7. †*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).

8. 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).

9. Voltage-controlled magnetic anisotropy in antiferromagnetic MgO-capped MnPt films: P. -H. Chang, W. Fang, T. Ozaki and K. D. Belashchenko, Phys. Rev. Materials **5**, 054406 (2021).

10. *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).

11. †*DCore: Integrated DMFT software for correlated electrons: H. Shinaoka, J. Otsuki, M. Kawamura, N. Takemori and K. Yoshimi, SciPost Phys. **10**, 117 (2021).

12. A structure map for AB2 type 2D materials using high-throughput DFT calculations: M. Fukuda, J. Zhang, Y. -T. Lee and T. Ozaki, Mater. Adv. **2**, 4392-4413 (2021).

Noguchi group

We have studied (1) reaction-diffusion waves on a deformable vesicle, (2) binding of isotropic curvature-inducing proteins onto membranes, (3) non-thermal fluctuations of membrane pushed by filament growth, (4) cavitation in Karman vortex of polymer solution, (5) fracture dynamics of polymer material, and (6) dynamics of water molecules on lipid membrane.

1. †Effects of polymers on the cavitating flow around a cylinder: A large-scale molecular dynamics analysis: Y. Asano, H. Watanabe and H. Noguchi, J. Chem. Phys. **155**, 014905 (2021).

2. 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).

3. Vesicle budding induced by binding of curvature-inducing proteins: H. Noguchi, Phys. Rev. E **104**, 014410 (2021).

4. Rotational Dynamics of Water at the Phospholipid Bilayer Depending on the Head Groups Studied by Molecular Dynamics Simulations: Y. Higuchi, Y. Asano, T. Kuwahara and M. Hishida, Langmuir **37**, 5329 (2021).

5. Three-Phase Coexistence in Binary Charged Lipid Membranes in a Hypotonic Solution: J. Guo, H. Ito, Y. Higuchi, K. Bohinc, N. Shimokawa and M. Takagi, Langmuir **37**, 9683 (2021).

6. Binding of curvature-inducing proteins onto tethered vesicles: H. Noguchi, Soft Matter **17**, 10469-10478 (2021).

7. Binding of thermalized and active membrane curvature-inducing proteins: Q. Goutaland, F. van Wijland, J.-B. Fournier and H. Noguchi, Soft Matter **17**, 5560-5573 (2021).

8. Reaction-diffusion waves coupled with membrane curvature: N. Tamemoto and H. Noguchi, Soft Matter **17**, 6589-6596 (2021).

---

* Joint research among groups within ISSP.

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

10. 荷電脂質膜の秩序形成：実験と粗視化分子動力学シミュレーションの融合：下川 直史 , 伊藤 弘明 , 樋口 祐次 , 分子シミュレーション学会誌「アンサンブル」**23**, 253-259 (2021).

11. Hydrophobic immiscibility controls self-sorting or co-assembly of peptide amphiphiles: R. Wakabayashi, R. Imatani, M. Katsuya, Y. Higuchi, H. Noguchi, N. Kamiya and M. Goto, Chem. Commun. **58**, 585 (2022).

12. Anisotropic, Degradable Polymer Assemblies Driven by a Rigid Hydrogen-Bonding Motif That Induce Shape-Specific Cell Responses: K. Fukushima, K. Matsuzaki, M. Oji, Y. Higuchi, G. Watanabe, Y. Suzuki, M. Kikuchi, N. Fujimura, N. Shimokawa, H. Ito, T. Kato, S. Kawaguchi and M. Tanaka, Macromolecules **55**, 15 (2022).

13. Nonequilibrium dynamics of a fluid vesicle: Turing patterns and traveling waves: H. Noguchi and N. Tamemoto, J. Phys.: Conf. Ser. **2207**, 012017 (2022).

14. †Binding of anisotropic curvature-inducing proteins onto membrane tubes: H. Noguchi, C. Tozzi and M. Arroyo, Soft Matter **18**, 3384--3394 (2022).

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 2021 include functional and usability enhancement of (1) 2DMAT and (2) RISM. We published four papers about the developed software packages (DCore, DSQSS, Kω, and RESPACK) in PASUMS. In addition, using these software packages, we have studied electronic properties of organic conductors β'-$[Pd(dmit)_2]_2$ and relaxation phenomena observed in quantum dot system. We also published the paper about the improvement of an analytic continuation method by combining sparse modeling with Pade approximation.

1. †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).

2. *Preparation and Readout of Multielectron High-Spin States in a Gate-Defined GaAs/AlGaAs Quantum Dot: H. Kiyama, K. Yoshimi, T. Kato, T. Nakajima, A. Oiwa and S. Tarucha, Phys. Rev. Lett. **127**, 086802(1-6) (2021).

3. †*DSQSS: Discrete Space Quantum Systems Solver: Y. Motoyama, K. Yoshimi, A. Masaki-Kato, T. Kato and N. Kawashima, Comput. Phys. Commun. **264**, 107944(1-9) (2021).

4. †*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).

5. †*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).

6. *Ab initio* derivation and exact diagonalization analysis of low-energy effective Hamiltonians for β′−[Pd(dmit)2]2: K. Yoshimi, T. Tsumuraya and T. Misawa, Phys. Rev. Research **3**, 043224 (2021).

7. †*DCore: Integrated DMFT software for correlated electrons: H. Shinaoka, J. Otsuki, M. Kawamura, N. Takemori and K. Yoshimi, SciPost Phys. **10**, 117 (2021).

8. Robust analytic continuation combining the advantages of the sparse modeling approach and the Padé approximation: Y. Motoyama, K. Yoshimi and J. Otsuki, Phys. Rev. B **105**, 035139 (2022).

9. *Unconventional dual 1D–2D quantum spin liquid revealed by ab initio studies on organic solids family: K. Ido, K. Yoshimi, T. Misawa and M. Imada, npj Quantum Mater. **7**, 48 (2022).

Neutron Science Laboratory

Yamamuro group

† Joint research with outside partners.

Our laboratory is studying chemical physics of complex condensed matters by using neutron scattering, X-ray diffraction, calorimetric, dielectric, and viscoelastic techniques. Our target materials are glasses, liquids, and various disordered systems. Following the vapor-deposited (VD) CS_2 and CCl_4 glasses, which were measured in 2018 and 2020, the inelastic neutron scattering (INS) experiment of VD H_2O glass (amorphous ice) was performed using AMATERAS in J-PARC MLF. By combining these three INS data , we have found a general relation between the low-energy excitations and local structures of glasses. The boson peak appears independently of the local structure, while the dispersive phonon excitations adjacent to the boson peak strongly depends on quasi-network structures of glasses (network formation degree: $H_2O > CCl_4 > CS_2$). The neutron diffraction (ND) of a novel hydrogen-cluster material Li_5MoD_{11} was measured on NOVA in J-PARC MLF. The Rietveld and pair distribution function (PDF) analyses revealed that the MoD_9 cluster is orientationally disordered down to 10 K, being consistent with the previous quasielastic neutron scattering (QENS) experiments. A ND work on amorphous D_2 deuterate was conducted on NOVA. The corresponding QENS work on amorphous H_2 hydrate was also performed using DNA and AGNES in JRR-3 which was restarted in 2021 after the long shutdown due to the Great East-Japan Earthquake in 2011. Other than these neutron works, the synchrotron-radiation X-ray diffraction works of toluene and glycerol liquids were carried out at high pressure up 4 GPa and room temperature using a Paris-Edinburgh cell and BL37XU at SPring-8. At higher pressures, we found drastic development in intermolecular correlation for toluene and more compact intramolecular structure keeping hydrogen bonds for glycerol.

1. 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).

2. Spin glass behavior and magnetic boson peak in a structural glass of a magnetic ionic liquid: M. Kofu, R. Watanuki, T. Sakakibara, S. Ohira-Kawamura, K. Nakajima, M. Matsuura, T. Ueki, K. Akutsu and O. Yamamuro, Sci. Rep. **11**, 12098 (2021).

3. Quasielastic neutron scattering study on proton dynamics assisted by water and ammonia molecules confined in MIL-53: S. Miyatsu, M. Kofu, A. Shigematsu, T. Yamada, H. Kitagawa, W. Lohstroh, G. Simeoni, M. Tyagi and O. Yamamuro, Structural Dynamics **8**, 054501 (2021).

4. Intermolecular correlations of liquid and glassy CS_2 studied by synchrotron radiation x-ray diffraction: Y. Mizuno, Y. Zhao, H. Akiba, S. Kohara, K. Ohara, M. G. Tucker, M. T. McDonnell and O. Yamamuro, J. Chem. Phys. **156**, 034503 (2022).

5. Structure of water-in-salt and water-in-bisalt electrolytes: M. A. González, H. Akiba, O. Borodin, G. J. Cuello, L. Hennet, S. Kohara, E. J. Maginn, L. Mangin-Thro, O. Yamamuro, Y. Zhang, D. L. Price and M. -L. Saboungi, Phys. Chem. Chem. Phys. **24**, 10727-10736 (2022).

6. 熱測定・中性子散乱による液晶性イオン液体のナノ構造とダイナミクス研究：根本 文也 , 古府 麻衣子 , 山室 修 , 日本液晶学会誌 **25(4)**, 230-236 (2021).

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; Nontrivial temperature dependence of magnetic anisotropy in multiferroic $Ba_2MnGe_2O_7$,magnetic diffuse scattering of $YBaCo_4O_7$ and $LuBaCo_4O_7$ on Kagome and triangular lattices, crystalline electric field level scheme of non-centrosymmetric $CeRhSi_3$ and $CeIrSi_3$, etc.

1. Antiferromagnetic Kitaev interaction in Jeff = 1/2 cobalt honeycomb materials $Na_3Co_2SbO_6$ and $Na_2Co_2TeO_6$: C. Kim, J. Jeong, G. Lin, P. Park, T. Masuda, S. Asai, S. Itoh, H.-S. Kim, H. Zhou, J. Ma and J.-G. Park, J. Phys.: Condens. Matter **34**, 045802(1-11) (2021).

2. Complex Magnetic Phase Diagram in the Non-Centrosymmetric Compound $CePtSi_3$: D. Ueta, M. Yoshida, T. Kobuke, Y. Ikeda, T. Masuda and H. Yoshizawa, J. Phys. Soc. Jpn. **90**, 064712(1-4) (2021).

3. Crystalline Electric Field Level Scheme of Non-centrosymmetric $CeRhSi_3$ and $CeIrSi_3$: D. Ueta, T. Kobuke, H. Shibata, M. Yoshida, Y. Ikeda, S. Itoh, T. Yokoo, T. Masuda and H. Yoshizawa, J. Phys. Soc. Jpn. **90**, 104706(1-7) (2021).

4. Magnetic Diffuse Scattering of $YBaCo_4O_7$ and $LuBaCo_4O_7$ on Kagome and Triangular Lattices: M. Soda, K. Morita, G. Ehlers, F. Ye, T. Tohyama, H. Yoshizawa, T. Masuda and H. Kawano-Furukawa, J. Phys. Soc. Jpn. **90**, 074704(1-5) (2021).

5. Oval-cycloidal Magnetic Structure with Phase-shift in the Non-centrosymmetric Tetragonal Compound $CePdSi_3$: D. Ueta, M. Yoshida, T. Kobuke, Y. Ikeda, A. Nakao, T. Moyoshi, K. Munakata, Y. Liu, T. Masuda and H. Yoshizawa, J.

* Joint research among groups within ISSP.

Phys. Soc. Jpn. **90**, 114702(1-5) (2021).

6. †*Spin-gap formation due to spin-Peierls instability in π-orbital-ordered NaO_2: M. Miyajima, F. Astuti, T. Fukuda, M. Kodani, S. Iida, S. Asai, A. Matsuo, T. Masuda, K. Kindo, T. Hasegawa, T. C. Kobayashi, T. Nakano, I. Watanabe and T. Kambe, Phys. Rev. B **104**, L140402(5) (2021).

7. †*Coexistence of Magnetoelectric and Antiferroelectric-like Orders in $Mn_3Ta_2O_8$: K. Kimura, N. Yagi, S. Hasegawa, M. Hagihala, A. Miyake, M. Tokunaga, H. Cao, T. Masuda and T. Kimura, Inorg. Chem. **60**, 15078(1-7) (2021).

8. Topological Analysis of the Experimental Electron Density in Multiferroic Antiferromagnet $Ba_2MnGe_2O_7$: R. Dutta, H. Thoma, D. Chernyshov, B. Nafradi, T. Masuda, A. Kriele and V. Hutanu, IEEE Trans. Magn. **58**, 2500206(1-6) (2021).

9. *Dimensional reduction by geometrical frustration in a cubic antiferromagnet composed of tetrahedral clusters: R. Okuma, M. Kofu, S. Asai, M. Avdeev, A. Koda, H. Okabe, M. Hiraishi, S. Takeshita, K. M. Kojima, R. Kadono, T. Masuda, K. Nakajima and Z. Hiroi, Nat. Commun. **12**, 4382(1-7) (2021).

10. 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).

11. Field-induced quantum spin disordered state in spin-1/2 honeycomb magnet $Na_2Co_2TeO_6$: G. Lin, J. Jeong, C. Kim, Y. Wang, Q. Huang, T. Masuda, S. Asai, S. Itoh, G. Günther, M. Russina, Z. Lu, J. Sheng, L. Wang, J. Wang, G. Wang, Q. Ren, C. Xi, W. Tong, L. Ling, Z. Liu, L. Wu, J. Mei, Z. Qu, H. Zhou, X. Wang, J.-G. Park, Y. Wan and J. Ma, Nat Commun **12**, 5559(1-8) (2021).

12. Triplon current generation in solids: Y. Chen, M. Sato, Y. Tang, Y. Shiomi, K. Oyanagi, T. Masuda, Y. Nambu, M. Fujita and E. Saitoh, Nat Commun **12**, 5199(1-7) (2021).

13. Nontrivial temperature dependence of magnetic anisotropy in multiferroic $Ba_2MnGe_2O_7$: S. Hasegawa, S. Hayashida, S. Asai, M. Matsuura, Z. Igor and T. Masuda, Phys. Rev. Research **3**, L032023(1-5) (2021).

14. Hybridized excitation of Higgs-amplitude and phase modes in frustrated quantum magnet: T. Masuda, S. Hayashida and M. Matsumoto, 日本物理学会誌 **76**, 23-27 (2021).

15. Novel Route for Analysis on Neutron Scattering Spectra: T. Masuda, JPSJ News Comments **18**, 03 (2021).

Nakajima group

Nakajima group has been studying magnetic materials showing cross-correlated phenomena related to topologically-nontrivial magnetic structures by means of neutron and X-ray scattering techniques. We are also responsible for a polarized-neutron triple-axis neutron spectrometer PONTA in the research reactor JRR-3 in Tokai. In this year, JRR-3 restarted its operation after the long shutdown since the east Japan great earthquake in 2011. We have updated components of the spectrometer and have supported the users who applied the joint-use user program of ISSP-NSL. One of the successful studies with the external users is the identification of complex magnetic orders in a centrosymmetric skyrmion host $EuAl_4$. Polarized neutron scattering at PONTA contributed to reveal successive magnetic phase transitions in this system at low temperatures in zero magnetic field. We are also collaborating with Kohama group in the international mega gauss laboratory in ISSP. By combining a long-pulse magnet developed by Kohama group with a pulsed neutron beam in J-PARC, we successfully performed time-of-flight neutron Laue diffraction measurements in long-pulse magnetic fields up to 14 T. We are planning to extend the limit of the magnetic field to 20-30 T in the future.

1. 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).

2. Robust noncoplanar magnetism in band-filling-tuned $(Nd_{1-x}Ca_x)_2Mo_2O_7$: M. Hirschberger, Y. Kaneko, L. Spitz, T. Nakajima, Y. Taguchi and Y. Tokura, Phys. Rev. B **104**, 024436 (2021).

3. Phase correction method in a wide detector plane for MIEZE spectroscopy with pulsed neutron beams: T. Oda, H. Endo, H. Ohshita, T. Seya, Y. Yasu, T. Nakajima, M. Hino and Y. Kawabata, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment **1012**, 165616 (2021).

4. †*Above-ordering-temperature large anomalous Hall effect in a triangular-lattice magnetic semiconductor: M. Uchida, S. Sato, H. Ishizuka, R. Kurihara, T. Nakajima, Y. Nakazawa, M. Ohno, M. Kriener, A. Miyake, K. Ohishi, T. Morikawa, M. S. Bahramy, T.-H. Arima, M. Tokunaga, N. Nagaosa and M. Kawasaki, Sci. Adv. **7**, eabl5381(1-8)

† Joint research with outside partners.

(2021).

5. Emergence of spin-orbit coupled ferromagnetic surface state derived from Zak phase in a nonmagnetic insulator FeSi: Y. Ohtsuka, N. Kanazawa, M. Hirayama, A. Matsui, T. Nomoto, R. Arita, T. Nakajima, T. Hanashima, V. Ukleev, H. Aoki, M. Mogi, K. Fujiwara, A. Tsukazaki, M. Ichikawa, M. Kawasaki and Y. Tokura, Sci. Adv. **7**, eabj0498 (2021).

6. Square and rhombic lattices of magnetic skyrmions in a centrosymmetric binary compound: R. Takagi, N. Matsuyama, V. Ukleev, L. Yu, J. S. White, S. Francoual, J. R. L. Mardegan, S. Hayami, H. Saito, K. Kaneko, K. Ohishi, Y. Onuki, T.-H. Arima, Y. Tokura, T. Nakajima and S. Seki, Nat Commun **13**, 1472 (2022).

7. Zoology of Multiple-*Q* Spin Textures in a Centrosymmetric Tetragonal Magnet with Itinerant Electrons: N. D. Khanh, T. Nakajima, S. Hayami, S. Gao, Y. Yamasaki, H. Sagayama, H. Nakao, R. Takagi, Y. Motome, Y. Tokura, T. Arima and S. Seki, Advanced Science **9**, 2105452 (2022).

Mayumi group

Mayumi group has discovered that slide-ring gels, in which polymer chains are cross-linked by ring molecules, show reversible strain-induced crystallization of polymer chains in loading/unloading process, which realizes their remarkable mechanical toughness and high recoverability under repeated cyclic deformation. The formation process of strain-induced crystalline structure has been probed by time-resolved scattering technique.

1. Tough hydrogels with rapid self-reinforcement: C. Liu, N. Morimoto, L. Jiang, S. Kawahara, T. Noritomi, H. Yokoyama, K. Mayumi and K. Ito, Science **372**, 1078 (2021).

2. Softness, Elasticity, and Toughness of Polymer Networks with Slide-Ring Cross-Links: K. Mayumi, C. Liu, Y. Yasuda and K. Ito, Gels **7**, 91 (2021).

3. Overscreening Induced by Ionic Adsorption at the Ionic Liquid/Electrode Interface Detected Using Neutron Reflectometry with a Rational Material Design: N. Nishi, J. Uchiyashiki, T. Oda, M. Hino and N. L. Yamada, Bulletin of the Chemical Society of Japan **94**, 2914-2918 (2021).

4. Tri-branched gels: Rubbery materials with the lowest branching factor approach the ideal elastic limit: T. Fujiyabu, N. Sakumichi, T. Katashima, C. Liu, K. Mayumi, U.-I. Chung and T. Sakai, Science Advances **8**, eabk0010 (2022).

International MegaGauss Science Laboratory

Kindo group

We have found better approach to produce the Cu-Ag wire for the pulsed magnet. We can not tell the better wire from good one by comparing tensile strength or conductivity but only by generating field. Good Cu-Ag wire can generate 75 Tesla(T) field without destruction but better one can 85 T. The wire produced by better approach generated the highest field up to 86.1 T in this year.

1. [*]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).

2. 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).

3. GdV_6Sn_6: A Multi-carrier Metal with Non-magnetic 3d-electron Kagome Bands and 4f-electron Magnetism: H. Ishikawa, T. Yajima, M. Kawamura, H. Mitamura and K. Kindo, J. Phys. Soc. Jpn. **90**, 124704(4) (2021).

4. 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).

5. [†*]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).

[*] Joint research among groups within ISSP.

6. Experimental determination of the magnetic interactions of frustrated Cairo pentagon lattice materials: M. D. Le, E. M. Wheeler, J. Jeong, K. Ramesh Kumar, S. Lee, C.-H. Lee, M. J. Oh, Y.-J. Jo, A. Kondo, K. Kindo, U. Stuhr, B. Fåk, M. Enderle, D. Batuk, A. M. Abakumov, A. A. Tsirlin and J.-G. Park, Phys. Rev. B **103**, 104423 (2021).

7. *Ferroelectric polarization reversal in multiferroic $MnWO_4$ via a rotating magnetic field up to 52 T: J. F. Wang, W. X. Liu, Z. Z. He, C. B. Liu, M. Tokunaga, M. Li, C. Dong, X. T. Han, F. Herlach, C. L. Lu, Z. W. Ouyang, Z. C. Xia, K. Kindo, L. Li and M. Yang, Phys. Rev. B **104**, 014415 (2021).

8. †*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).

9. †High magnetic field properties in $Ru_{2-x}Fe_xCrSi$ with antiferromagnetic and spin-glass states: M. Hiroi, S. Nishiinoue, I. Shigeta, M. Ito, K. Koyama, A. Kondo, K. Kindo, I. Watanabe, M. Fujii, S. Kimura, H. Manaka and N. Terada, Phys. Rev. B **103**, 094428 (2021).

10. *Normal state specific heat in the cuprate superconductors $La_{2-x}Sr_xCuO_4$ and $Bi_{2+y}Sr_{2-x-y}LaxCuO_{6+\delta}$ near the critical point of the pseudogap phase: C. Girod, D. LeBoeuf, A. Demuer, G. Seyfarth, S. Imajo, K. Kindo, Y. Kohama, M. Lizaire, A. Legros, A. Gourgout, H. Takagi, T. Kurosawa, M. Oda, N. Momono, J. Chang, S. Ono, G. -q. Zheng, C. Marcenat, L. Taillefer and T. Klein, Phys. Rev. B **103**, 214506 (2021).

11. *Phase transition in the 5d(1) double perovskite Ba_2CaReO_6 induced by high magnetic field: H. Ishikawa, D. Hirai, A. Ikeda, M. Gen, T. Yajima, A. Matsuo, Y. H. Matsuda, Z. Hiroi and K. Kindo, Phys. Rev. B **104**, 174422(7) (2021).

12. †*Physical properties of liquid oxygen under ultrahigh magnetic fields: T. Nomura, A. Ikeda, M. Gen, A. Matsuo, K. Kindo, Y. Kohama, Y. H. Matsuda, S. Zherlitsyn, J. Wosnitza, H. Tsuda and T. C. Kobayashi, Phys. Rev. B **104**, 224423(10) (2021).

13. †*Quantum antiferromagnet bluebellite comprising a maple-leaf lattice made of spin-1/2 Cu^{2+} ions: Y. Haraguchi, A. Matsuo, K. Kindo and Z. Hiroi, Phys. Rev. B **104**, 174439(6) (2021).

14. *Quantum transport of topological spin solitons in a one-dimensional organic ferroelectric: S. Imajo, A. Miyake, R. Kurihara, M. Tokunaga, K. Kindo, S. Horiuchi and F. Kagawa, Phys. Rev. B **103**, L201117 (2021).

15. †*Spin-gap formation due to spin-Peierls instability in π-orbital-ordered NaO_2: M. Miyajima, F. Astuti, T. Fukuda, M. Kodani, S. Iida, S. Asai, A. Matsuo, T. Masuda, K. Kindo, T. Hasegawa, T. C. Kobayashi, T. Nakano, I. Watanabe and T. Kambe, Phys. Rev. B **104**, L140402(5) (2021).

16. 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).

17. Thermodynamic evidence for the formation of a Fulde-Ferrell-Larkin-Ovchinnikov phase in the organic superconductor $\lambda-(BETS)_2GaCl_4$: S. Imajo, T. Kobayashi, A. Kawamoto, K. Kindo and Y. Nakazawa, Phys. Rev. B **103**, L220501 (2021).

18. The FFLO State in the Dimer Mott Organic Superconductor κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br: S. Imajo and K. Kindo, Crystals **11**, 1358(11) (2021).

19. Ni deficiency effects on martensitic phase transition in Ni_2MnGa: M. Ito, S. Kuwahara, A. Taira, H. Matsuguma, A. Kondo and K. Kindo, Physica B: Condensed Matter **611**, 412794 (2021).

20. *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).

21. *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).

22. †*Nuclear magnetic resonance measurements in dynamically controlled field pulse: Y. Ihara, K. Hayashi, T. Kanda, K. Matsui, K. Kindo and Y. Kohama, Review of Scientific Instruments **92**, 114709(8) (2021).

23. *Extraordinary π-electron superconductivity emerging from a quantum spin liquid: S. Imajo, S. Sugiura, H. Akutsu, Y. Kohama, T. Isono, T. Terashima, K. Kindo, S. Uji and Y. Nakazawa, Phys. Rev. Research **3**, 033026 (2021).

24. *Revealing three-dimensional quantum criticality by Sr substitution in Han purple: S. Allenspach, P. Puphal, J. Link, I. Heinmaa, E. Pomjakushina, C. Krellner, J. Lass, G. S. Tucker, C. Niedermayer, S. Imajo, Y. Kohama, K. Kindo, S. Kramer, M. Horvatic, M. Jaime, A. Madsen, A. Mira, N. Laflorencie, F. Mila, B. Normand, C. Ruegg, R. Stern and F. Weickert, Phys. Rev. Research **3**, 023177 (2021).

† Joint research with outside partners.

25. †*Nature of field-induced antiferromagnetic order in Zn-doped $CeCoIn_5$ and its connection to quantum criticality in the pure compound: M. Yokoyama, Y. Honma, Y. Oshima, ?. Rahmanto, K. Suzuki, K. Tenya, Y. Shimizu, D. Aoki, A. Matsuo, K. Kindo, S. Nakamura, Y. Kono, S. Kittaka and T. Sakakibara, Phys. Rev. B **105**, 054515(9) (2022).

26. Optical selection rules of the magnetic excitation in the S=1/2 one-dimensional Ising-like antiferromagnet $BaCo_2V_2O_8$: S. Kimura, H. Onishi, A. Okutani, M. Akaki, Y. Narumi, M. Hagiwara, K. Okunishi, K. Kindo, Z. He, T. Taniyama and M. Itoh, Phys. Rev. B **105**, 014417(9) (2022).

27. Reentrant ferroelectric phase induced by a tilting high magnetic field in $Ni_3V_2O_8$: C. Dong, J. F. Wang, Z. Z. He, Y. T. Chang, M. Y. Shi, Y. R. Song, S. M. Jin, Y. Q. Du, Z. Y. Wu, X. T. Han, K. Kindo and M. Yang, Phys. Rev. B **105**, 024427(6) (2022).

28. †Revised phase diagram of the high-T_c cuprate superconductor Pb-doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ revealed by anisotropic transport measurements: K. Harada, Y. Teramoto, T. Usui, K. Itaka, T. Fujii, T. Noji, H. Taniguchi, M. Matsukawa, H. Ishikawa, K. Kindo, D. S. Dessau and T. Watanabe, Phys. Rev. B **105**, 085131(9) (2022).

29. †Quantum paramagnetism in the hyperhoneycomb Kitaev magnet $\beta-ZnIrO_3$: Y. Haraguchi, A. Matsuo, K. Kindo and H. A. Katori, Phys. Rev. Materials **6**, L021401(6) (2022).

30. †Spin-glass transition in the spin–orbit-entangled Jeff=0 Mott insulating double-perovskite ruthenate: H. Yatsuzuka, Y. Haraguchi, A. Matsuo, K. Kindo and H. A. Katori, Sci Rep **12**, 2429(6) (2022).

Tokunaga group

The topological Hall effect, which reflects the scalar spin chirality produced by magnetic ordering, was studied in various magnetic materials. Our experiments on magnetotransport properties in high magnetic fields have revealed that the anomalous Hall effect grows at high temperatures after arriving at a forced ferromagnetic state in some magnetic materials. Such phenomena suggest a new mechanism for the giant anomalous Hall effect.

1. †Anisotropic Physical Properties of Layered Antiferromagnet $U_2Pt_6Ga_{15}$: Y. Matsumoto, Y. Haga, E. Yamamoto, T. Takeuchi, A. Miyake and M. Tokunaga, J. Phys. Soc. Jpn. **90**, 074707(1-6) (2021).

2. Enhancement and Discontinuity of Effective Mass through the First-Order Metamagnetic Transition in UTe_2: A. Miyake, Y. Shimizu, Y. J. Sato, D. Li, A. Nakamura, Y. Homma, F. Honda, J. Flouquet, M. Tokunaga and D. Aoki, J. Phys. Soc. Jpn. **90**, 103702(1-5) (2021).

3. †*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).

4. *Ferroelectric polarization reversal in multiferroic $MnWO_4$ via a rotating magnetic field up to 52 T: J. F. Wang, W. X. Liu, Z. Z. He, C. B. Liu, M. Tokunaga, M. Li, C. Dong, X. T. Han, F. Herlach, C. L. Lu, Z. W. Ouyang, Z. C. Xia, K. Kindo, L. Li and M. Yang, Phys. Rev. B **104**, 014415 (2021).

5. †*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).

6. †*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).

7. Quantum transport observed in films of the magnetic topological semimetal $EuSb_2$: M. Ohno, M. Uchida, R. Kurihara, S. Minami, Y. Nakazawa, S. Sato, M. Kriener, M. Hirayama, A. Miyake, Y. Taguchi, R. Arita, M. Tokunaga and M. Kawasaki, Phys. Rev. B **103**, 165144(1-6) (2021).

8. *Quantum transport of topological spin solitons in a one-dimensional organic ferroelectric: S. Imajo, A. Miyake, R. Kurihara, M. Tokunaga, K. Kindo, S. Horiuchi and F. Kagawa, Phys. Rev. B **103**, L201117 (2021).

9. †*Magnetoconduction in the Correlated Semiconductor FeSi in Ultrastrong Magnetic Fields up to a Semiconductor-to-Metal Transition: D. Nakamura, Y. H. Matsuda, A. Ikeda, A. Miyake, M. Tokunaga, S. Takeyama and T. Kanomata, Phys. Rev. Lett. **127**, 156601 (1-6) (2021).

10. †*Coexistence of Magnetoelectric and Antiferroelectric-like Orders in $Mn_3Ta_2O_8$: K. Kimura, N. Yagi, S. Hasegawa, M. Hagihala, A. Miyake, M. Tokunaga, H. Cao, T. Masuda and T. Kimura, Inorg. Chem. **60**, 15078(1-7) (2021).

11. †Enhancing Thermopower and Nernst Signal of High-Mobility Dirac Carriers by Fermi Level Tuning in the Layered

* Joint research among groups within ISSP.

Magnet $EuMnBi_2$: K. Tsuruda, K. Nakagawa, M. Ochi, K. Kuroki, M. Tokunaga, H. Murakawa, N. Hanasaki and H. Sakai, Adv. Funct. Mater. **31**, 2102275 (2021).

12. †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).

13. †*Above-ordering-temperature large anomalous Hall effect in a triangular-lattice magnetic semiconductor: M. Uchida, S. Sato, H. Ishizuka, R. Kurihara, T. Nakajima, Y. Nakazawa, M. Ohno, M. Kriener, A. Miyake, K. Ohishi, T. Morikawa, M. S. Bahramy, T.-H. Arima, M. Tokunaga, N. Nagaosa and M. Kawasaki, Sci. Adv. **7**, eabl5381(1-8) (2021).

14. †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).

15. †Restoration of the collinear spin arrangement in non-magnetic-ion-substituted M-type hexaferrite by high magnetic fields: K. Kamishima, A. Yonezawa, K. Kakizaki, A. Miyake, H. Mitamura and M. Tokunaga, Journal of Magnetism and Magnetic Materials **538**, 168251(1-5) (2021).

16. †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).

17. Molecular beam deposition of a new layered pnictide with distorted Sb square nets: M. Ohno, M. Uchida, Y. Nakazawa, S. Sato, M. Kriener, A. Miyake, M. Tokunaga, Y. Taguchi and M. Kawasaki, APL Materials **9**, 051107(1-4) (2021).

18. †Tunable spin-valley coupling in layered polar Dirac metals: M. Kondo, M. Ochi, T. Kojima, R. Kurihara, D. Sekine, M. Matsubara, A. Miyake, M. Tokunaga, K. Kuroki, H. Murakawa, N. Hanasaki and H. Sakai, Commun Mater **2**, 49(1-7) (2021).

19. Elastic Soft Mode and Electric Quadrupole Response in Excitonic Insulator Candidate $(Ta_{0.952}V_{0.048})_2NiSe_5$: Contribution of Electron–Phonon Interaction: R. Kurihara, Y. Hirose, S. Sano, K. Mitsumoto, A. Miyake, M. Tokunaga and R. Settai, J. Phys. Soc. Jpn. **91**, 024601(1-7) (2022).

20. †Magnetism of $Al_xFe_{2-x}GeO_5$ with Andalusite Structure: K. Kakimoto, S. Takada, H. Ohta, Y. Haraguchi, M. Hagihala, S. Torii, T. Kamiyama, H. Mitamura, M. Tokunaga, A. Hatakeyama and H. A. Katori, J. Phys. Soc. Jpn. **91**, 054704(1-7) (2022).

21. Extremely high upper critical field in $BiCh_2$-based (Ch: S and Se) layered superconductor $LaO_{0.5}F_{0.5}BiS_{2-x}Se_x$ (x = 0.22 and 0.69): K. Hoshi, R. Kurihara, Y. Goto, M. Tokunaga and Y. Mizuguchi, Sci Rep **12**, 288(1-8) (2022).

22. †Field-induced multiple metal-insulator crossovers of correlated Dirac electrons of perovskite $CaIrO_3$: R. Yamada, J. Fujioka, M. Kawamura, S. Sakai, M. Hirayama, R. Arita, T. Okawa, D. Hashizume, T. Sato, F. Kagawa, R. Kurihara, M. Tokunaga and Y. Tokura, npj Quantum Mater. **7**, 13(1-6) (2022).

Y. Matsuda group

The magnetic-field-induced insulator-metal transition in the correlated narrow gap semiconductor FeSi has been investigated using ultrahigh magnetic fields of up to 500 T generated by the electromagnetic flux compression technique. The critical magnetic field of the phase transition is found to be 270 T. It is found that the ingap state plays an important role in the mechanism of magnetoresistance in high magnetic fields. Closing of the energy gap due to the Zeeman shift of the electronic bands explains the metallization in an ultrahigh magnetic field. As for the single-turn coil technique, a development of the techniques for the generation of high magnetic fields has been made. A change in the weight of the single-turned coil affects the process of the magnetic field generation and the maximum magnetic field increases with increasing the weight. Another important technical development has been made for the ultrasound experiment and the technique has been applied for the study of liquid oxygen up to 140 T. The ultrasound experiment of Kondo insulator YbB_{12} has been performed in a relatively lower field range up to 60 T. Although the quantum oscillation has not been observed in the response of the ultrasound, the anomalous magnetic field dependence of the elastic constants was found at temperatures around 30 K, which suggests the magnetic-field-induced valence fluctuation of Yb ions.

1. †*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).

2. *Phase transition in the 5d(1) double perovskite Ba_2CaReO_6 induced by high magnetic field: H. Ishikawa, D. Hirai, A.

† Joint research with outside partners.

Ikeda, M. Gen, T. Yajima, A. Matsuo, Y. H. Matsuda, Z. Hiroi and K. Kindo, Phys. Rev. B **104**, 174422(7) (2021).

3. †*Physical properties of liquid oxygen under ultrahigh magnetic fields: T. Nomura, A. Ikeda, M. Gen, A. Matsuo, K. Kindo, Y. Kohama, Y. H. Matsuda, S. Zherlitsyn, J. Wosnitza, H. Tsuda and T. C. Kobayashi, Phys. Rev. B **104**, 224423(10) (2021).

4. †*Magnetoconduction in the Correlated Semiconductor FeSi in Ultrastrong Magnetic Fields up to a Semiconductor-to-Metal Transition: D. Nakamura, Y. H. Matsuda, A. Ikeda, A. Miyake, M. Tokunaga, S. Takeyama and T. Kanomata, Phys. Rev. Lett. **127**, 156601 (1-6) (2021).

5. †*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).

6. *Ultrasound measurement technique for the single-turn-coil magnets: T. Nomura, A. Hauspurg, D. I. Gorbunov, A. Miyata, E. Schulze, S. A. Zvyagin, V. Tsurkan, Y. H. Matsuda, Y. Kohama and S. Zherlitsyn, Review of Scientific Instruments **92**, 063902(8) (2021).

7. *Ferroelectric Transition of a Chiral Molecular Crystal BINOL·2DMSO: T. Nomura, T. Yajima, Z. Yang, R. Kurihara, Y. Ishii, M. Tokunaga, Y. H. Matsuda, Y. Kohama, K. Kimura and T. Kimura, J. Phys. Soc. Jpn. **91**, 064702 (2022).

8. Generating 77 T using a portable pulse magnet for single-shot quantum beam experiments: A. Ikeda, Y. H. Matsuda, X. Zhou, S. Peng, Y. Ishii, T. Yajima, Y. Kubota, I. Inoue, Y. Inubushi, K. Tono and M. Yabashi, Appl. Phys. Lett. **120**, 142403 5pages (2022).

Kohama group

We have investigated various high-field properties. In $Pb(TiO)Cu_4(PO_4)_4$, Sn(SeS), and $MAPbX_3$ (X = I, Br, and Cl), the field induced phenomena have been investigated by magnetooptics in non-destructive and destructive magnetic fields. In $Ba_{0.9}Sr_{0.1}CuSi_2O$, graphite, and high-T_c superconductor, we have used specific heat and MCE techniques. The TDO and resistivity measurements have revealed rich transport phenomena in two dimensional materials, such as KZnBi and organic conductors. We have developed NMR measurement technique for measuring spin-lattice and spin-spin relaxation rates in pulsed magnetic fields. We also have developed the ultrasound experiemnt technique for investigations in destructive pulsed fields. We are now constructing new apparatus for the neutron scattering experiment in long pulse fields.

1. *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).

2. 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).

3. Nonreciprocal Directional Dichroism in a Magnetic-Field-Induced Ferroelectric Phase of $Pb(TiO)Cu_4(PO_4)_4$: T. Katsuyoshi, K. Kimura, Z. Yang, Y. Kato, S. Kimura, Y. Motome, Y. Kohama and T. Kimura, J. Phys. Soc. Jpn. **90**, 123701 (2021).

4. Combination of optical transitions of polarons with Rashba effect in methylammonium lead trihalide perovskites under high magnetic fields: Y. H. Shin, H. Choi, C. Park, D. Park, M. S. Jeong, H. Nojiri, Z. Yang, Y. Kohama and Y. Kim, Phys. Rev. B **104**, 035205 (2021).

5. 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).

6. Heavy carrier effective masses in van der Waals semiconductor Sn(SeS) revealed by high magnetic fields up to 150 T: Z. Yang, X. Wang, J. Felton, Z. Kudrynskyi, M. Gen, T. Nomura, X. Wang, L. Eaves, Z. D. Kovalyuk, Y. Kohama, L. Zhang and A. Patanè, Phys. Rev. B **104**, 085206 (2021).

7. *Normal state specific heat in the cuprate superconductors $La_{2-x}Sr_xCuO_4$ and $Bi_{2+y}Sr_{2-x-y}LaxCuO_{6+\delta}$ near the critical point of the pseudogap phase: C. Girod, D. LeBoeuf, A. Demuer, G. Seyfarth, S. Imajo, K. Kindo, Y. Kohama, M. Lizaire, A. Legros, A. Gourgout, H. Takagi, T. Kurosawa, M. Oda, N. Momono, J. Chang, S. Ono, G. -q. Zheng, C. Marcenat, L. Taillefer and T. Klein, Phys. Rev. B **103**, 214506 (2021).

8. †*Physical properties of liquid oxygen under ultrahigh magnetic fields: T. Nomura, A. Ikeda, M. Gen, A. Matsuo,

* Joint research among groups within ISSP.

K. Kindo, Y. Kohama, Y. H. Matsuda, S. Zherlitsyn, J. Wosnitza, H. Tsuda and T. C. Kobayashi, Phys. Rev. B **104**, 224423(10) (2021).

9. 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).

10. *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).

11. †*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).

12. *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).

13. †*Nuclear magnetic resonance measurements in dynamically controlled field pulse: Y. Ihara, K. Hayashi, T. Kanda, K. Matsui, K. Kindo and Y. Kohama, Review of Scientific Instruments **92**, 114709(8) (2021).

14. *Ultrasound measurement technique for the single-turn-coil magnets: T. Nomura, A. Hauspurg, D. I. Gorbunov, A. Miyata, E. Schulze, S. A. Zvyagin, V. Tsurkan, Y. H. Matsuda, Y. Kohama and S. Zherlitsyn, Review of Scientific Instruments **92**, 063902(8) (2021).

15. Tunable Berry curvature and transport crossover in topological Dirac semimetal KZnBi: J. Song, B. C. Park, K. I. Sim, J. Bang, S. Kim, Z. Yang, Y. Kohama, Y. Kim and S. W. Kim, npj Quantum Mater. **6**, 77 (2021).

16. *Extraordinary π-electron superconductivity emerging from a quantum spin liquid: S. Imajo, S. Sugiura, H. Akutsu, Y. Kohama, T. Isono, T. Terashima, K. Kindo, S. Uji and Y. Nakazawa, Phys. Rev. Research **3**, 033026 (2021).

17. *Revealing three-dimensional quantum criticality by Sr substitution in Han purple: S. Allenspach, P. Puphal, J. Link, I. Heinmaa, E. Pomjakushina, C. Krellner, J. Lass, G. S. Tucker, C. Niedermayer, S. Imajo, Y. Kohama, K. Kindo, S. Kramer, M. Horvatic, M. Jaime, A. Madsen, A. Mira, N. Laflorencie, F. Mila, B. Normand, C. Ruegg, R. Stern and F. Weickert, Phys. Rev. Research **3**, 023177 (2021).

18. *Ferroelectric Transition of a Chiral Molecular Crystal BINOL·2DMSO: T. Nomura, T. Yajima, Z. Yang, R. Kurihara, Y. Ishii, M. Tokunaga, Y. H. Matsuda, Y. Kohama, K. Kimura and T. Kimura, J. Phys. Soc. Jpn. **91**, 064702 (2022).

19. Quantum phase of the chromium spinel oxide $HgCr_2O_4$ in high magnetic fields: S. Kimura, S. Imajo, M. Gen, T. Momoi, M. Hagiwara, H. Ueda and Y. Kohama, Phys. Rev. B **105**, L180405 (2022).

Center of Computational Materials Science

Akai group

(1) The temperature dependence of intrinsic magnetic properties is one of the most important ingredients that determine the final performance of permanent magnets. In view of this, we have developed the methods that enable us to evaluate the magnetic properties under the influence of electron-magnon and electron-phonon scattering. (2) The hyperfine field distributions in the vicinity of the interface of Fe/MgO epitaxial films was detected layer by layer measurement using synchrotron Mössbauer source. We compare the experimental results with the first-principles calculation using KKR-CPA combined the optimized effective potential (OEP) method. The calculated hyperfine interactions provides important information about the electronic and lattice structure at the interfaces. (3) We have developed the method that enables us to calculate spin-wave dispersion and exchange stiffness of metallic magnet from first-principles. The exchange interactions between local spin density are calculated by Liechtenstein's method in the momentum space. The spin-wave dispersions are then directly calculated by diagonalizing the low energy effective Hamiltonian. (4) A new data assimilation methods that assimilate experimental and theoretical data obtained for permanent magnet materials. Based on a general framework for constructing a predictor from two data sets including missing values, a practical scheme for magnetic materials is formulated in which a small number of experimental data in limited composition space are integrated with a larger number of first-principles calculation data. Using this scheme we have evaluated the finite-temperature magnetization of permanent magnets over a high-dimensional composition space.

1. 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).

† Joint research with outside partners.

2. Direct observation of magnetic Friedel oscillation at Fe(001) surface: T. Mitsui, S. Sakai, S. Li, T. Ueno, T. Watanuki, Y. Kobayashi, R. Masuda, M. Seto and H. Akai, Hyperfine Interact **242**, 37 (2021).

3. 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).

4. Atomistic theory of thermally activated magnetization processes in $Nd_2Fe_{14}B$ pemanent magnet: S. Miyashita, M. Nishino, Y. Toga, T. Hinokihara, I. E. Uysal, T. Miyake, H. Akai, S. Hirosawa and A. Sakuma, Science and Technology of Advanced Materials **22**, 658–682 (2021).

5. Understanding and optimization of hard magnetic compounds from first principles: T. Miyake, Y. Harashima, T. Fukazawa and H. Akai, Science and Technology of Advanced Materials **22**, 543–556 (2021).

6. 鉄の表面近傍の特異な磁性を発見—原子一層毎に磁気モーメントの大きさが増減する : 三井 隆也 , 境誠 司 , 瀬戸 誠 , 赤井 久純 , 日本物理学会誌 **77**, 23-28 (2022).

7. First-principles investigation of Nd(Fe,M)$_{12}$ (M=k–Br) and Nd(Fe,Cr,Co,Ni,Ge,As): Possible enhancers of Curie temperature for $NdFe_{12}$ magnetic compounds: T. Fukazawa, H. Akai, Y. Harashima and T. Miyake, Acta Materialia **226**, 117597 (2022).

8. *Automatic exhaustive calculations of large material space by Korringa-Kohn-Rostoker coherent potential approximation method — Applied to equiatomic quaternary high entropy alloys: T. Fukushima, H. Akai, T. Chikyow and H. Kino, Pays. Rev. Mater. **6**, 023802(1-19) (2022).

Laser and Synchrotron Research Center

Kobayashi group

We are developing state-of-the-art laser system for laser processing and breath diagnosis. Process informatics is a new target to study.

1. *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).

2. レーザー加工の学理探索とデータ科学 : 小林 洋平 , 精密工学会誌 **87**, 601 (2021).

3. Independent contribution of optical attenuation length in ultrafast laser-induced structural change: T. Shibuya, K. Sakaue, H. Ogawa, D. Satoh, T.-H. Dinh, M. Ishino, M. Tanaka, M. Washio, T. Higashiguchi, M. Nishikino, A. Kon, Y. Kubota, Y. Inubushi, S. Owada, Y. Kobayashi and R. Kuroda, Opt. Express **29**, 33121 (2021).

4. 次世代レーザー及び加工の共通基盤技術開発 : 中里 智治 , レーザー加工学会誌 **10**, 135 (2021).

5. 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).

6. †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).

7. †Fully Automated Data Acquisition for Laser Production Cyber-Physical System: Y. Kobayashi, T. Takahashi, T. Nakazato, H. Sakurai, H. Tamaru, K. Ishikawa, K. Sakaue and S. Tani, IEEE J. Select. Topics Quantum Electron. **27**, 1 (2021).

8. レーザー加工 CPS 開発 : 坂上 和之 , 田丸 博晴 , 小林 洋平 , オプトロニクス **9**, 74 (2021).

9. † 次世代のモノづくり拠点を目指すレーザー加工プラットフォームとデータベース : 中里 智治 , 高塚 肇 , 西林 一彦 , 田丸 博晴 , 小林 洋平 , 湯本 潤司 , オプトロニクス **3**, 91 (2021).

10. Autonomous parameter optimization for femtosecond laser micro-drilling: K. Bamoto, H. Sakurai, S. Tani and Y. Kobayashi, Opt. Express **30**, 243 (2022).

11. Ultrafast laser ablation simulator using deep neural networks: S. Tani and Y. Kobayashi, Sci Rep **12**, 5837 (2022).

* Joint research among groups within ISSP.

12. Fiber lasers: Z. Z. K. Y. J. S, in: *Handbook of Laser Micro- and Nano-Engineering*, edited by Koji Sugioka, (Springer nature Switzerland, 2021), 1-32.

Harada group

We are developing instrumentation and exploring novel applications of soft X-ray emission spectroscopy in preparation for the next generation of synchrotron radiation. We discussed the segmented cross undulator as a novel polarization-controlled light source. Additionally, a soft X-ray CMOS image sensor with a wide dynamic range (WDR) is proposed (sxCMOS). We detected fully spin-polarized electronic states in the buried magnetic layer of Co_2MnSi, a prototype of semi-metallic Heusler alloys, using RIXS-MCD, as a pioneering application of the newly developed analytical approach. The minority-spin Fe-3d impurity band (IB) in (In,Fe)As, a typical n-type FMS, was studied using soft X-ray angle-resolved photoemission spectroscopy (SX-ARPES). The itinerant/localized nature of distinct dd excitations in TiO_2 nanocrystals with lattice multiphase was revealed by RIXS measurements on both Ti and O sites. In addition, various solutions and solid-liquid interfaces were investigated by RIXS. An isolated water molecule strongly interacting with an Li ion in a new high-salt concentration aqueous electrolyte solution "hydrate melt" was identified by RIXS and first-principles molecular dynamics simulation. RIXS of colloidal dispersions of multi-walled carbon nanotubes treated by solution plasma revealed the reconstruction of hydrogen-bonded network of water via orbital hybridization with the oxygen-containing functional groups generated by plasma treatment. In addition, we analyzed water encapsulated in the loop-shaped polyethylene glycol chain brushes and observed the absence of entropically-favored tetrahedrally coordinated water, which possibly regulates the biocompatibility.

1. †Minority-spin impurity band in n-type (In,Fe)As: A materials perspective for ferromagnetic semiconductors: M. Kobayashi, L. D. Anh, J. Minar, W. Khan, S. Borek, P. N. Hai, Y. Harada, T. Schmitt, M. Oshima, A. Fujimori, M. Tanaka and V. N. Strocov, Phys. Rev. B **103**, 115111 (1-10) (2021).

2. †Soft X-ray Emission Studies on Hydrate-Melt Electrolytes: T. Shimada, N. Takenaka, E. Watanabe, Y. Yamada, Y.-T. Cui, Y. Harada, M. Okubo and A. Yamada, J. Phys. Chem. B **125**, 11534-11539 (2021).

3. †Soft X-ray emission spectroscopy for the electronic state of water molecules influenced by plasma-treated multi-walled carbon nanotubes: N. Sakakibara, K. Inoue, S. Takahashi, T. Goto, T. Ito, K. Akada, J. Miyawaki, Y. Hakuta, K. Terashima and Y. Harada, Phys. Chem. Chem. Phys. **23**, 10468-10474 (2021).

4. A Global Shutter Wide Dynamic Range Soft X-Ray CMOS Image Sensor With Backside- Illuminated Pinned Photo-diode, Two-Stage Lateral Overflow Integration Capacitor, and Voltage Domain Memory Bank: H. Shike, R. Kuroda, R. Kobayashi, M. Murata, Y. Fujihara, M. Suzuki, S. Harada, T. Shibaguchi, N. Kuriyama, T. Hatsui, J. Miyawaki, T. Harada, Y. Yamasaki, T. Watanabe, Y. Harada and S. Sugawa, IEEE Trans. Electron Devices **68**, 2056-2063 (2021).

5. †Detecting halfmetallic electronic structures of spintronic materials in a magnetic field: H. Fujiwara, R. Y. Umetsu, F. Kuroda, J. Miyawaki, T. Kashiuchi, K. Nishimoto, K. Nagai, A. Sekiyama, A. Irizawa, Y. Takeda, Y. Saitoh, T. Oguchi, Y. Harada and S. Suga, Sci Rep **11**, 18654 (1-9) (2021).

6. †*Fast and versatile polarization control of X-ray by segmented cross undulator at SPring-8: J. Miyawaki, S. Yamamoto, Y. Hirata, M. Horio, Y. Harada and I. Matsuda, AAPPS Bull. **31**, 25-1,-24 (2021).

7. †Hydrogen-Bonded Structure of Water in the Loop of Anchored Polyrotaxane Chain Controlled by Anchoring Density: K. Akada, K. Yamazoe, J. Miyawaki, R. Maeda, K. Ito and Y. Harada, Front. Chem. **9**, 743255 (1-8) (2021).

8. †Electronic surface reconstruction of TiO_2 nanocrystals revealed by resonant inelastic x-ray scattering: C.-H. Chuang, C.-M. Chen, Y.-C. Shao, P.-H. Yeh, C.-M. Chang, W.-F. Pong, M. Kapilashrami, P.-A. Glans, S. Gul, G. Wang, Y. Li, J. Zhang, J. Miyawaki, H. Niwa, Y. Harada, J.-M. Chen and J. Guo, Journal of Vacuum Science & Technology A **39**, 063204 (1-6) (2021).

9. †The Near Future of Synchrotron Radiation Operando Analysis : Development of Soft X-ray Absorption and Emission Spectroscopy for Functional Materials: Y. HARADA, Journal of the Japan Society for Precision Engineering **87**, 34-38 (2021).

10. † 放射光軟 X 線分光法によるリチウムイオン電池の電子状態オペランド計測 : 細野 英司 , 原田 慈久 , 朝倉 大輔 , 計測と制御 **60**, 207-212 (2021).

11. † 高分子内に入り込んだ水の電子状態観測 : 倉橋 直也 , 山添 康介 ,「【水】と機能性ポリマーに関する材料設計・最新応用」, 第 2 章 第 2 節 ,（株）技術情報協会 企画編集 , (（株）技術情報協会 , 2021), 42-52.

I. Matsuda group

† Joint research with outside partners.

The global pandemics of coronavirus disease (COVID-19) continued in 2021. We carried out research and user-supports with care at the beamline, SPring-8 BL07LSU. Since a project of the next-generation synchrotron radiation facility was launched, we participated devotedly in the construction and started technical developments, such as nano-focusing and scanning measurements. In the laboratory, we have succeeded in updating the soft X-ray non-linear optical effect into a spectroscopic method for materials science at X-ray free electron laser facility at SACLA.

1. Atomic arrangements of quasicrystal bilayer graphene: Interlayer distance expansion: Y. Fukaya, Y. Zhao, H.-W. Kim, J. R. Ahn, H. Fukidome and I. Matsuda, Phys. Rev. B **104**, L180202(1-5) (2021).

2. Polarization-Resolved Extreme-Ultraviolet Second-Harmonic Generation from $LiNbO_3$: C. B. Uzundal, S. Jamnuch, E. Berger, C. Woodahl, P. Manset, Y. Hirata, T. Sumi, A. Amado, H. Akai, Y. Kubota, S. Owada, K. Tono, M. Yabashi, J. W. Freeland, C. P. Schwartz, W. S. Drisdell, I. Matsuda, T. A. Pascal, A. Zong and M. Zuerch, Phys. Rev. Lett. **127**, 237402(1-8) (2021).

3. † ビスマス薄膜を通して「見る」表面物理学の新展開 : 伊藤 俊 , 松田 巌 , 日本物理学会誌 **76**, 566-574 (2021).

4. Recent Progress in Spectroscopies Using Soft X-ray Free-electron Lasers: I. Matsuda and Y. Kubota, Chem. Lett. **50**, 1336-1344 (2021).

5. †*Band Bending of n-GaN under Ambient H_2O Vapor Studied by X-ray Photoelectron Spectroscopy: Y. Imazeki, M. Sato, T. Takeda, M. Kobayashi, S. Yamamoto, I. Matsuda, J. Yoshinobu, M. Sugiyama and Y. Nakano, J. Phys. Chem. C **125**, 9011 (2021).

6. †*Comparative Study of H_2O and O_2 Adsorption on the GaN Surface: M. Sato, Y. Imazeki, T. Takeda, M. Kobayashi, S. Yamamoto, I. Matsuda, J. Yoshinobu, Y. Nakano and M. Sugiyama, J. Phys. Chem. C **125**, 25807 (2021).

7. †*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).

8. Influence of Stacking Order of Phthalocyanine and Fullerene Layers on the Photoexcited Carrier Dynamics in Model Organic Solar Cell: K. Ozawa, S. Yamamoto, T. Miyazawa, K. Yano, K. Okudaira, K. Mase and I. Matsuda, J. Phys. Chem. C **125**, 13963-13970 (2021).

9. Extreme Ultraviolet Second Harmonic Generation Spectroscopy in a Polar Metal: E. Berger, S. Jamnuch, C. B. Uzundal, C. Woodahl, H. Padmanabhan, A. Amado, P. Manset, Y. Hirata, Y. Kubota, S. Owada, K. Tono, M. Yabashi, C. Wang, Y. Shi, V. Gopalan, C. P. Schwartz, W. S. Drisdell, I. Matsuda, J. W. Freeland, T. A. Pascal and M. Zuerch, Nano Lett. **21**, 6095-6101 (2021).

10. A novel measurement approach for near-edge x-ray absorption fine structure: Continuous 2 π angular rotation of linear polarization: Y. Kudo, Y. Hirata, M. Horio, M. Niibe and I. Matsuda, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment **1018**, 165804(1-5) (2021).

11. †Electronic structure of a borophene layer in rare-earth aluminum/chromium boride and its hydrogenated derivative borophane: M. Niibe, M. Cameau, N. T. Cuong, O. I. Sunday, X. Zhang, Y. Tsujikawa, S. Okada, K. Yubuta, T. Kondo and I. Matsuda, Phys. Rev. Materials **5**, 084007-1,-8 (2021).

12. †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**, 20-23 (2021).

13. *Ultrafast optical stress on $BaFe_2As_2$: T. Suzuki, Y. Kubota, A. Nakamura, T. Shimojima, K. Takubo, S. Ito, K. Yamamoto, S. Michimae, H. Sato, H. Hiramatsu, H. Hosono, T. Togashi, M. Yabashi, H. Wadati, I. Matsuda, S. Shin and K. Okazaki, Phys. Rev. Research **3**, 033222 (2021).

14. †*Fast and versatile polarization control of X-ray by segmented cross undulator at SPring-8: J. Miyawaki, S. Yamamoto, Y. Hirata, M. Horio, Y. Harada and I. Matsuda, AAPPS Bull. **31**, 25(1-24) (2021).

15. *Environmental effects on layer-dependent dynamics of Dirac fermions in quasicrystalline bilayer graphene: Y. Zhao, T. Suzuki, T. Iimori, H. -W. Kim, J. R. Ahn, M. Horio, Y. Sato, Y. Fukaya, T. Kanai, K. Okazaki, S. Shin, S. Tanaka, F. Komori, H. Fukidome and I. Matsuda, Phys. Rev. B **105**, 115304 (2022).

16. *Photoinduced transient states of antiferromagnetic orderings in $La_{1/3}Sr_{2/3}FeO_3$ and $SrFeO_{3-\delta}$ thin films observed through time-resolved resonant soft x-ray scattering: K. Yamamoto, T. Tsuyama, S. Ito, K. Takubo, I. Matsuda, N. Pontius, C. Schüßler-Langeheine, M. Minohara, H. Kumigashira, Y. Yamasaki, H. Nakao, Y. Murakami, T. Katase, T.

* Joint research among groups within ISSP.

Kamiya and H. Wadati, New J. Phys. **24**, 043012(1-9) (2022).

17. †*Functionalization of the MoS_2 basal plane for activation of molecular hydrogen by Pd deposition: F. Ozaki, S. Tanaka, W. Osada, K. Mukai, M. Horio, T. Koitaya, S. Yamamoto, I. Matsuda and J. Yoshinobu, Applied Surface Science **593**, 153313 (2022).

18. †*Hydrogen absorption and diffusion behaviors in cube-shaped palladium nanoparticles revealed by ambient-pressure X-ray photoelectron spectroscopy: J. Tang, O. Seo, D. S. R. Rocabado, T. Koitaya, S. Yamamoto, Y. Nanba, C. Song, J. Kim, A. Yoshigoe, M. Koyama, S. Dekura, H. Kobayashi, H. Kitagawa, O. Sakata, I. Matsuda and J. Yoshinobu, Applied Surface Science **587**, 152797 (2022).

19. Separating Non-linear Optical Signals of a Sample from High Harmonic Radiation in a Soft X-ray Free Electron Laser: T. Sumi, M. Horio, T. Senoo, T. Wada, Y. Tsujikawa, X. Zhang, P. Manset, M. Araki, Y. Hirata, W. S. Drisdell, J. W. Freeland, A. Amado, M. Zuerch, Y. Kubota, S. Owada, K. Tono, M. Yabashi, C. P. Schwartz and I. Matsuda, e-J. Surf. Sci. Nanotechnol. **20**, 31(1-5) (2022).

20. Electronic Structures of Polymorphic Layers of Borophane: I. Tateishi, X. Zhang and I. Matsuda, Molecules **27**, 1808(1-13) (2022).

21. †Measurement of X-ray Magnetic Linear Dichroism by Rotating Polarization Angle of Soft X-ray Generated by a Segmented Undulator: Y. Kudo, M. Horio, Y. Hirata, T. Ohkochi, T. Kinoshita and I. Matsuda, e-Journal of Surface Science and Nanotechnology (2022), accepted for publication.

22. 2D boron: Boraphene, Borophene, Boronene: I. Matsuda and K. Wu ed., (Springer Nature, Switzerland, 2021).

23. 物理科学，この 1 年　2022: 松田 巌 , 近藤 剛弘他 , (丸善出版 , 東京都千代田区 , 2022).

Itatani group

Advancements in soft x-ray attosecond spectroscopy and attosecond beamlines were also continued. First, quantum mechanical simulation revealed that the 2ω oscillations observed in a triatomic molecule (N_2O) arise from tunnel ionization of core-excited states, leading to a new understanding of transient absorption spectroscopy using soft x-ray attosecond pulses. Second, a water flat-jet system was developed for transient soft X-ray spectroscopy of liquids and solvents. High-order harmonics coupled with molecular vibrations were observed upon irradiation of intense mid-infrared pulses. Further experiments are now underway to elucidate molecular dynamics. Third, high-field electron scattering experiments were performed, and the cutoff behavior was successfully discussed in terms of quantum theory. Finally, a new infrared parametric light source using a Yb-based solid-state laser was developed, and phase-stable sub-30 fs pulses were obtained at repetition rates of 10 kHz and 100 kHz. In addition, a Yb-based solid-state laser was used to generate 6-eV pulses for angle-resolved photoemission spectroscopy.

1. *High-harmonic generation in GaAs beyond the perturbative regime: P. Xia, T. Tamaya, C. Kim, F. Lu, T. Kanai, N. Ishii, J. Itatani, H. Akiyama and T. Kato, Phys. Rev. B **104**, L121202(1-6) (2021).

2. †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).

3. *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).

4. †Time-domain spectroscopy of optical parametric amplification for phase-stable terahertz-to-midinfrared pulses: N. Kanda, N. Ishii, J. Itatani and R. Matsunaga, Optics Express **29(3)**, 3479-3489 (2021).

5. †Magnetic Domain Control of $ErFeO_3$ by Intense Terahertz Free Electron Laser Pulses: M. Nakajima, G. Isoyama and T. Kurihara, IEEE Trans. on Plasma Sci **49**, 3344-3350 (2021).

6. Attosecond electronic dynamics of core-excited states of N_2O in the soft x-ray region,: N. Saito, N. Douguet, H. Sannohe, N. Ishii, T. Kanai, Y. Wu, A. Chew, S. Han, B. I. Schneider, J. Olsen, L. Argenti, Z. Chang and J. Itatani, Phys. Rev. Res. **3**, 043222(1-8) (2021).

7. *Photo-Excitation Band-Structure Engineering of 2*H*-$NbSe_2$ Probed by Time- and Angle-Resolved Photoemission Spectroscopy: M. Watanabe, T. Suzuki, T. Someya, Y. Ogawa, S. Michimae, M. Fujisawa, T. Kanai, J. Itatani, T. Saitoh, S. Shin and K. Okazaki, J. Phys. Soc. Jpn. **91**, 064703 (2022).

8. †Ultrafast multidimensional spectroscopy with field resolution and noncollinear geometry at mid-infrared frequencies: T. Deckert, J. Allerbeck, T. Kurihara and D. Brida, New J. Phys. **24**, 023005(1-9) (2022).

† Joint research with outside partners.

9. †Spin canting in nonlinear terahertz magnon dynamics revealed by magnetorefractive probing in orthoferrite: T. Kurihara, M. Bamba, H. Watanabe, M. Nakajima and T. Suemoto, arXiv **2202**, 11365 (2022).

Kondo group

We gave the evidence for a higher-order topological insulator in a three-dimensional material built from van der Waals stacking of bismuth-halide chains and visualized the strain-induced topological phase transition in a quasi-one-dimensional superconductor $TaSe_3$.

1. Reduced Hall carrier density in the overdoped strange metal regime of cuprate supercond.: C. Putzke, S. Benhabib, W. Tabis, J. Ayres, Z. Wang, L. Malone, S. Licciardello, J. Lu, T. Kondo, T. Takeuchi, N. E. Hussey, J. R. Cooper and A. Carrington, Nature Phys. **17**, 826-831 (2021).
2. *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).
3. Anomalous vortex liquid in charge-ordered cuprate superconductors: Y.-T. Hsu, M. Berben, M. culo, S. Adachi, T. Kondo, T. Takeuchi, Y. Wang, S. Wiedmann, S. M. Hayden and N. E. Hussey, Proc. Natl. Acad. Sci. U.S.A. **118**, e2016275118(1-6) (2021).
4. *Evidence for a higher-order topological insulator in a three-dimensional material built from van der Waals stacking of bismuth-halide chains: R. Noguchi, M. Kobayashi, Z. Jiang, K. Kuroda, T. Takahashi, Z. Xu, D. Lee, M. Hirayama, M. Ochi, T. Shirasawa, P. Zhang, C. Lin, C. Bareille, S. Sakuragi, H. Tanaka, S. Kunisada, K. Kurokawa, K. Yaji, A. Harasawa, V. Kandyba, A. Giampietri, A. Barinov, T. K. Kim, C. Cacho, M. Hashimoto, D. Lu, S. Shin, R. Arita, K. Lai, T. Sasagawa and T. Kondo, Nature Materials **20**, 473-479 (2021).
5. *Visualization of the strain-induced topological phase transition in a quasi-one-dimensional superconductor $TaSe_3$: C. Lin, M. Ochi, R. Noguchi, K. Kuroda, M. Sakoda, A. Nomura, M. Tsubota, P. Zhang, C. Bareille, K. Kurokawa, Y. Arai, K. Kawaguchi, H. Tanaka, K. Yaji, A. Harasawa, M. Hashimoto, D. Lu, S. Shin, R. Arita, S. Tanda and T. Kondo, Nature Materials **20**, 1093-1099 (2021).
6. *Scaling law for Rashba-type spin splitting in quantum-well films: R. Noguchi, K. Kuroda, M. Kawamura, K. Yaji, A. Harasawa, T. Iimori, S. Shin, F. Komori, T. Ozaki and T. Kondo, Phys. Review B **103**, 180409(1-6) (2021).
7. *Multipole polaron in the devil's staircase of CeSb: Y. Arai, K. Kuroda, T. Nomoto, Z. H. Tin, S. Sakuragi, C. Bareille, S. Akebi, K. Kurokawa, Y. Kinoshita, W. -L. Zhang, S. Shin, M. Tokunaga, H. Kitazawa, Y. Haga, H. S. Suzuki, S. Miyasaka, S. Tajima, K. Iwasa, R. Arita and T. Kondo, Nat. Mater. **21**, 410(1-7) (2022).
8. Large anomalous Hall effect induced by weak ferromagnetism in the noncentrosymmetric antiferromagnet $CoNb_3S_6$: H. Tanaka, S. Okazaki, K. Kuroda, R. Noguchi, Y. Arai, S. Minami, S. Ideta, K. Tanaka, D. Lu, M. Hashimoto, V. Kandyba, M. Cattelan, A. Barinov, T. Muro, T. Sasagawa and T. Kondo, Phys. Review B **105**, 121102(1-7) (2022).
9. *Selective observation of surface and bulk bands in polar WTe_2 by laser-based spin- and angle-resolved photoemission spectroscopy.: Y. Wan, L. Wang, K. Kuroda, P. Zhang, K. Koshiishi, M. Suzuki, J. Kim, R. Noguchi, C. Bareille, K. Yaji, A. Harasawa, S. Shin, S.-W. Cheong, A. Fujimori and T. Kondo, Phys. Review B **105**, 085421 (2022).
10. *Visualization of optical polarization transfer to photoelectron spin vector emitted from a spin-orbit coupled surface state.: K. Kuroda, K. Yaji, R. Noguchi, A. Harasawa, S. Shin, T. Kondo and F. Komori, Phys. Review B **105**, 121106(1-6) (2022).

Matsunaga group

We have investigated light-matter interactions and light-induced nonequilibrium phenomena in solids by utilizing terahertz (THz) pulse. By using a Yb-based laser system and the multiplate broadening scheme, we realized phase-stable broadband multiterahertz pulses (10-45 THz, 40-180 meV, or 7-30 μm) with the pulse width of 28 fs. By using the multiterahertz pulse for time-resolved detection of complex response functions, we have investigated ultrafast dynamics of the photoexcited electrons in a 3D Dirac semimetal Cd_3As_2. We also demonstrate that a large reduction of the refractive index by 80% dominates the nonequilibrium infrared response of the Dirac semimetal, which can be utilized for designing ultrafast switches in active optoelectronics.

1. * ワイル反強磁性金属 Mn_3Sn 薄膜の室温テラヘルツ異常ホール効果 : 松田 拓也 , 肥後 友也 , 神田 夏輝 , 松永 隆佑 , 応

* Joint research among groups within ISSP.

用物理 **90**, 752 (2021).

2. テラヘルツパルス技術で拓く物性物理学と新奇機能性 : 松永 隆佑 , レーザー研究 **49**, 325 (2021).

3. *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).

4. Topological Materials for Functional Optoelectronic Devices: H. Chorsi, B. Cheng, B. Zhao, J. Toudert, V. Asadchy, O. F. Shoron, S. Fan and R. Matsunaga, Advanced Functional Materials **32**, 2110655 (2022).

5. *Tracking Ultrafast Change of Multiterahertz Broadband Response Functions in a Photoexcited Dirac Semimetal Cd_3As_2 Thin Film: N. Kanda, Y. Murotani, T. Matsuda, M. Goyal, S. Salmani-Rezaie, J. Yoshinobu, S. Stemmer and R. Matsunaga, Nano Letters **22**, 2358 (2022).

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 2021, we have revealed the two-fold symmetric superconducting gap of $FeSe_{0.78}S_{0.22}$ irrespective of its four-fold symmetric crystal structure by high-resolution laser ARPES. In addition, we have revealed a characteristic electron-phonon coupling during the photo-induced insulator-to-metal transition in 1*T*-TaS_2 from the FDARPES measurements by using HHG laser time-resolved ARPES.

1. *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).

2. *Ultrafast optical stress on $BaFe_2As_2$: T. Suzuki, Y. Kubota, A. Nakamura, T. Shimojima, K. Takubo, S. Ito, K. Yamamoto, S. Michimae, H. Sato, H. Hiramatsu, H. Hosono, T. Togashi, M. Yabashi, H. Wadati, I. Matsuda, S. Shin and K. Okazaki, Phys. Rev. Research **3**, 033222 (2021).

3. Discovery of Pressure-Induced Superconductivity in an Excitonic Insulator: K. Okazaki, JPSJ News Comments **18**, 11 (2021).

4. *Photo-Excitation Band-Structure Engineering of 2*H*-$NbSe_2$ Probed by Time- and Angle-Resolved Photoemission Spectroscopy: M. Watanabe, T. Suzuki, T. Someya, Y. Ogawa, S. Michimae, M. Fujisawa, T. Kanai, J. Itatani, T. Saitoh, S. Shin and K. Okazaki, J. Phys. Soc. Jpn. **91**, 064703 (2022).

5. *Environmental effects on layer-dependent dynamics of Dirac fermions in quasicrystalline bilayer graphene: Y. Zhao, T. Suzuki, T. Iimori, H. -W. Kim, J. R. Ahn, M. Horio, Y. Sato, Y. Fukaya, T. Kanai, K. Okazaki, S. Shin, S. Tanaka, F. Komori, H. Fukidome and I. Matsuda, Phys. Rev. B **105**, 115304 (2022).

6. HHG-laser-based time- and angle-resolved photoemission spectroscopy of quantum materials: T. Suzuki, S. Shin and K. Okazaki, Journal of Electron Spectroscopy and Related Phenomena **251**, 147105 (2021).

Kimura group

In FY2021, the Kimura group worked on the development of in-situ imaging techniques for mixing reactions of solution samples using the X-ray free-electron laser at SACLA and microscopic imaging techniques using soft X-rays at BL07LSU of SPring-8. In the experiment at SACLA, we succeeded in imaging nanoparticle structures in a mixed solution at sub-10-nanometer resolution; in the experiment at SPring-8 BL07LSU, we constructed a soft x-ray ptychography system using total-reflection Wolter mirror optics.

1. Copper electroforming replication process for soft x-ray mirrors: G. Yamaguchi, H. Motoyama, S. Owada, Y. Kubota, S. Egawa, T. Kume, Y. Takeo, M. Yabashi and H. Mimura, Review of Scientific Instruments **92**, 123106 (2021).
2. Current status of development of electroforming process for high precision soft x-ray mirrors: T. Kume, G. Yamaguchi, K. Hiraguri, Y. Matsuzawa, Y. Imamura, H. Miyashita, T. Saito, Y. Takeo, Y. Senba, H. Kishimoto, H. Ohashi, H. Hashizume, H. Mimura, C. Morawe, A. M. Khounsary and S. Goto, Proc. of SPIE **11837**(1-5) (2021).
3. Development of figure correction system for axisymmetric x-ray mirrors: S. Yokomae, Y. Takeo, T. Shimamura, Y. Matsuzawa, T. Kume, Y. Senba, H. Kishimoto, H. Ohashi, H. Mimura, C. Morawe, A. M. Khounsary and S. Goto, Proc. of SPIE **11837**(1-7) (2021).
4. Electrodeposition simulation for fabricating Wolter mirrors of x-ray telescopes: A. Ito, G. Yamaguchi, T. Watanabe, Y.

† Joint research with outside partners.

Takeo, T. Kume, Y. Matsuzawa, T. Saito, K. Hiraguri, K. Tamura, A. Takigawa, T. Kanoh, N. Ishida, I. Mitsuishi, H. Hashizume, H. Mimura, C. Morawe, A. M. Khounsary and S. Goto, Proc. of SPIE **11837**(1-9) (2021).
5. An arrayed-window microfluidic device for observation of mixed nanoparticles with an X-ray free-electron laser: Y. Matsumoto, Y. Takeo, S. Egawa, G. Yamaguchi, S. Yokomae, M. Takei, H. Yumoto, T. Koyama, H. Ohashi, K. Tono, M. Yabashi, H. Mimura and T. Kimura, Opt Rev **29**, 7 (2022).

* Joint research among groups within ISSP.