

# Publications

# ISSP publications

## 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 2024 are to develop (1) the high conductive EDOT [(3,4-ethylenedioxythiophene)]-based oligomer conductors by the introduction of Se atoms and (2) the Ni dithiolene-based flexible capsules with uniaxial magnetic anisotropy in water.

1. オリゴマー型有機電子材料の高伝導化: 藤野 智子, 小野塚 洗太, 森初 果, 応用物理 **93**, 490-493 (2024).
2.  $t^*$ Orbital hybridization of donor and acceptor to enhance the conductivity of mixed-stack complexes: T. Fujino, R. Kameyama, K. Onozuka, K. Matsuo, S. Dekura, T. Miyamoto, Z. Guo, H. Okamoto, T. Nakamura, K. Yoshimi, S. Kitou, T.-H. Arima, H. Sato, K. Yamamoto, A. Takahashi, H. Sawa, Y. Nakamura and H. Mori, Nat Commun **15**, 3028 (2024).
3.  $t^*$ Combined x-ray diffraction, electrical resistivity, and *ab initio* study of (TMTTF)<sub>2</sub>PF<sub>6</sub> under pressure: Implications for the unified phase diagram: M. Itoi, K. Yoshimi, H. Ma, T. Misawa, T. Tsumuraya, D. Bhoi, T. Komatsu, H. Mori, Y. Uwatoko and H. Seo, Phys. Rev. Research **6**, 043308 (1-14) (2024).
4. \*Higher conductivity in doped ethylenedioxythiophene (EDOT) dimers with chalcogen-substituted end groups: K. Onozuka, T. Fujino, T. Miyamoto, T. Yamakawa, H. Okamoto, H. Akiba, O. Yamamuro, E. Kayahara, S. Yamago, H. Oike and H. Mori, J. Mater. Chem. C **12**, 13956 (2024).
5. Single-crystalline oligomer-based conductors modeling the doped poly(3,4-ethylenedioxythiophene) family: T. Fujino, R. Kameyama, K. Onozuka, K. Matsuo, S. Dekura, K. Yoshimi and H. Mori, Faraday Discuss. **250**, 348 (2024).
6. \*Discovery of bicyclic borane molecule B<sub>14</sub>H<sub>26</sub>: X. Zhang, T. Fujino, Y. Ando, Y. Tsujikawa, T. Wang, T. Nakashima, H. Sakurai, K. Yamaguchi, M. Horio, H. Mori, J. Yoshinobu, T. Kondo and I. Matsuda, Commun Chem **8**, 14 (2025).
7. \*Macroscopic Structural Transition of Nickel Dithiolate Capsule with Uniaxial Magnetic Anisotropy in Water: T. Fujino, M. Hishida, M. Ito, T. Nakamura, M. Asada, N. Kurahashi, H. Kiuchi, Y. Harada, K. Harano, R. Makiura, K. J. Takeno, S. Yokomori, H. Oike and H. Mori, Adv. Science (2025), accepted for publication.
8. 高性能かつ大気安定なアンバイポーラ型分子性半導体材料の開発: 藤野 智子, 伊藤 雅聡, 森 初果, 「有機半導体の開発と最新動向」, 監修: 安達千波矢, (シーエムシー出版, 2024), 154-163.

### Osada group

We have studied the tight-binding model for the  $\alpha$ -type layered organic conductors,  $\alpha$ -(ET)<sub>2</sub>I<sub>3</sub> and  $\alpha$ -(BETS)<sub>2</sub>I<sub>3</sub>, with a uniform interlayer coupling accompanied by spin-orbit interaction originating from the I<sub>3</sub><sup>-</sup> anion potential. The model preserves the time reversal and inversion symmetries. In  $\alpha$ -(ET)<sub>2</sub>I<sub>3</sub>, the interlayer spin-orbit coupling realizes the experimentally suggested Dirac semimetal state with inversion symmetry. In contrast, the inversion breaking in interlayer hoppings realizes the Weyl semimetal state without spin-orbit coupling. In  $\alpha$ -(BETS)<sub>2</sub>I<sub>3</sub>, the proposed strong topological insulator is hardly realized with inversion symmetry.

1. Hofstadter Butterfly and Broken-Symmetry Quantum Hall States in  $\alpha$ -Type Organic Dirac Fermion Systems: T. Osada, J. Phys. Soc. Jpn. **93**, 034711(1-6) (2024).
2. Three-Dimensional Topological Semimetal/Insulator States in  $\alpha$ -Type Organic Conductors with Interlayer Spin-Orbit Interaction: T. Osada, J. Phys. Soc. Jpn. **93**, 123703(1-4) (2024).

## 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) low-temperature magnetostriction measurements of a quantum spin ice candidate  $\text{Ce}_2\text{Hf}_2\text{O}_7$  (2) spontaneous thermal Hall measurements of candidate materials of chiral superconductivity, and (3) thermal Hall measurements of kagome antiferromagnets.

1. Doping-tunable Fermi surface with persistent topological Hall effect in the axion candidate  $\text{EuIn}_2\text{As}_2$ : J. Yan, J. Si, Z. Jiang, H. Ma, Y. Uwatoko, B.-T. Wang, X. Luo, Y. Sun and M. Yamashita, *Phys. Rev. B* **110**, 115111 (2024).
2. Magnetic structure of polar magnet  $\text{GaV}_4\text{Se}_8$  with Neél-type skyrmion lattice probed by  $^{51}\text{V}$  NMR: H. Takeda, M. Ishikawa, M. Takigawa, M. Yamashita, Y. Fujima and T.-H. Arima, *Phys. Rev. B* **110**, 224430 (2024).
3.  $*J_{\text{eff}} = 1/2$  Hyperoctagon Lattice in Cobalt Oxalate Metal-Organic Framework: H. Ishikawa, S. Imajo, H. Takeda, M. Kakegawa, M. Yamashita, J.-I. Yamaura and K. Kindo, *Phys. Rev. Lett.* **132**, 156702 (2024).
4. Incommensurate magnetic order in an axion insulator candidate  $\text{EuIn}_2\text{As}_2$  investigated by NMR measurement: H. Takeda, J. Yan, Z. Jiang, X. Luo, Y. Sun and M. Yamashita, *npj Quantum Mater.* **9**, 67 (2024).
5. Magnon thermal Hall effect via emergent  $\text{SU}(3)$  flux on the antiferromagnetic skyrmion lattice: H. Takeda, M. Kawano, K. Tamura, M. Akazawa, J. Yan, T. Waki, H. Nakamura, K. Sato, Y. Narumi, M. Hagiwara, M. Yamashita and C. Hotta, *Nature Communications* **15**, 566 (2024).
6.  $^{\dagger}$ Rotational Grüneisen ratio: A probe for quantum criticality in anisotropic systems: S. Yuasa, Y. Kono, Y. Ozaki, M. Yamashita, Y. Shimura, T. Takabatake and S. Kittaka, *Phys. Rev. B* **111**, 045123 (2025).

## Ideue group

We have explored novel transport and optical properties reflecting symmetry breaking in two-dimensional materials. We found that symmetry-reduced uniaxial-strained trigonal superconductor exhibits a superconducting diode effect. We also investigated nonlinear optical properties of symmetry-controlled van der Waals magnets. In particular, we revealed that complex magnetic symmetry and the resulting unique second harmonic generation can be realized at the heterointerface of two-dimensional magnets with different magnetic anisotropies.

1.  $*$ Gilbert damping of NiFe thin films grown on two-dimensional chiral hybrid lead-iodide perovskites: T. Hatajiri, S. Sakamoto, H. Kosaki, Z. Tian, M. Tanaka, T. Ideue, K. Inoue, D. Miyajima and S. Miwa, *Phys. Rev. B* **110**, 054435 (1-6) (2024).
2. Superconducting diode effect under time reversal symmetry: F. Liu, Y. M. Itahashi, S. Aoki, Y. Dong, Z. Wang, N. Ogawa, T. Ideue and Y. Iwasa, *Science Advances* **10**, eado1502 (2024).
3. Gate-Controlled Potassium Intercalation and Superconductivity in Molybdenum Disulfide: R. D. Septianto, A. P. Romagosa, Y. Dong, H. Matsuoka, T. Ideue, Y. Majima and Y. Iwasa, *Nano Letters* **24**, 13790-13795 (2024).
4. Giant Modulation of the Second Harmonic Generation by Magnetoelectricity in Two-Dimensional Multiferroic  $\text{CuCrP}_2\text{S}_6$ : S. Aoki, Y. Dong, Z. Wang, X. S. W. Huang, Y. M. Itahashi, N. Ogawa, T. Ideue and Y. Iwasa, *Advanced Materials* **36**, 2312781 (2024).

## Takagi group

This year we have reported spontaneous topological Hall effect induced by collinear antiferromagnetic order in altermagnet  $\text{FeS}$ . We also revealed multistep topological transitions in a tetragonal magnet  $\text{GdRu}_2\text{Ge}_2$  and spin excitations for skyrmion states in a polar magnet  $\text{VOSe}_2\text{O}_5$ .

1. SP-STM study of the multi-Q phases in  $\text{GdRu}_2\text{Si}_2$ : J. Spethmann, N. D. Khanh, H. Yoshimochi, R. Takagi, S. Hayami, Y. Motome, R. Wiesendanger, S. Seki and K. von Bergmann, *Phys. Rev. Materials* **8**, 064404 (2024).
2.  $*$ Multistep topological transitions among meron and skyrmion crystals in a centrosymmetric magnet: H. Yoshimochi, R. Takagi, J. Ju, N. D. Khanh, H. Saito, H. Sagayama, H. Nakao, S. Itoh, Y. Tokura, T. Arima, S. Hayami, T. Nakajima and S. Seki, *Nature Physics* **20**, 1001-1008 (2024).
3. Exotic Spin Excitations in a Polar Magnet  $\text{VOSe}_2\text{O}_5$ : T. Araki, R. Takagi, T. Kurumaji, Y. Tokura, M. Mochizuki and S. Seki, *Physical Review Letters* **133**, 136702 (2024).
4.  $*$ Spontaneous Hall effect induced by collinear antiferromagnetic order at room temperature: R. Takagi, R. Hirakida, Y. Settai, R. Oiwa, H. Takagi, A. Kitaori, K. Yamauchi, H. Inoue, J.-I. Yamaura, D. Nishio-Hamane, S. Itoh, S. Aji, H. Saito, T. Nakajima, T. Nomoto and R. A. & S. Seki, *Nature Materials* **24**, 63-68 (2025).

# Division of Condensed Matter Theory

## Tsunetsugu group

We have worked on a theoretical proposal for realizing long-period modulated structures of electronic degrees of freedom with even parity under time reversal operation. This includes various incommensurate orders of electric quadrupoles using electron's orbital degrees of freedom. We have demonstrated the presence of such an incommensurate phase realized on a triangular lattice. We have performed Monte Carlo simulations to investigate long range correlations based on its classical effective model, and found that it is a critical phase characterized by a Kosterlitz-Thouless type transition. We have also continued a study on basic properties of chiral phonons and now the target system is a three dimensional lattice with cubic symmetry.

1. Numerical Renormalization Group Study of Quadrupole Kondo Effect with the Crystal-Field Excited State: Y. Kaneko and H. Tsunetsugu, *J. Phys. Soc. Jpn.* **93**, 033705 (2024).
2. Orbital moire' and quadrupolar triple-q physics in a triangular lattice: K. Hattori, T. Ishitobi and H. Tsunetsugu, *Phys. Rev. Research* **6**, L042068-1-7 (2024).
3. Proof of Completeness of the Local Conserved Quantities in the One-Dimensional Hubbard Model: K. Fukai, *J Stat Phys* **191**, 70 (2024).
4. On correlation functions in models related to the Temperley-Lieb algebra: K. Fukai, R. Kleinemu"hl, B. Pozsgay and E. Vernier, *SciPost Phys.* **16**, 003 (2024).

## Kato group

The main research subject of Kato Lab. is transport properties in mesoscopic and spintronic devices. We theoretically studied nonequilibrium spin transport in the context of chiral phonons, material curvature, spin noises, thermal transport, and spin pumping.

1. Spin pumping into quantum spin chains: S. C. Furuya, M. Matsuo and T. Kato, *Phys. Rev. B* **110**, 165129(1-13) (2024).
2. Theory of the inverse Rashba-Edelstein effect induced by thermal spin injection: K. Hosokawa, M. Yama, M. Matsuo and T. Kato, *Phys. Rev. B* **110**, 035309(1-12) (2024).
3. Chirality-Induced Phonon-Spin Conversion at an Interface: T. Funato, M. Matsuo and T. Kato, *Phys. Rev. Lett.* **132**, 236201(1-7) (2024).
4. †\*Observation of Terahertz Spin Hall Conductivity Spectrum in GaAs with Optical Spin Injection: T. Fujimoto, T. Kurihara, Y. Murotani, T. Tamaya, N. Kanda, C. Kim, J. Yoshinobu, H. Akiyama, T. Kato and R. Matsunaga, *Phys. Rev. Lett.* **132**, 016301(1-7) (2024).
5. †\*Sub-photon accuracy noise reduction of a single shot coherent diffraction pattern with an atomic model trained autoencoder: T. Ishikawa, Y. Takeo, K. Sakurai, K. Yoshinaga, N. Furuya, Y. Inubushi, K. Tono, Y. Joti, M. Yabashi, T. Kimura and K. Yoshimi, *Opt. Express* **32**, 18301 (2024).
6. †\*H-wave – A Python package for the Hartree-Fock approximation and the random phase approximation: T. Aoyama, K. Yoshimi, K. Ido, Y. Motoyama, T. Kawamura, T. Misawa, T. Kato and A. Kobayashi, *Computer Physics Communications* **298**, 109087(1-10) (2024).
7. 国際物理オリンピック 2023 日本大会 理論問題作成の舞台裏: 加藤 岳生, *大学の物理教育* **30**, 10-13 (2024).
8. Curvature-induced valley-dependent spin-orbit interaction: A. Yamakage, T. Sato, R. Okuyama, T. Funato, W. Izumida, K. Sato, T. Kato and M. Matsuo, *Phys. Rev. B* **111**, 045121(1-12) (2025).
9. \*Light-induced inverse spin Hall effect and field-induced circular photogalvanic effect in GaAs revealed by two-dimensional terahertz Fourier analysis: T. Fujimoto, Y. Murotani, T. Tamaya, T. Kurihara, N. Kanda, C. Kim, J. Yoshinobu, H. Akiyama, T. Kato and R. Matsunaga, *Phys. Rev. B* **111**, L201201 (2025).
10. Microscopic theory of Rashba-Edelstein magnetoresistance: M. Yama, M. Matsuo and T. Kato, *Phys. Rev. B* **111**, 144416(1-20) (2025).
11. Fluctuations in Spin Dynamics Excited by Pulsed Light: T. Sato, S. Watanabe, M. Matsuo and T. Kato, *Phys. Rev. Lett.* **134**, 106702(1-7) (2025).
12. Theory of spin pumping and inverse Rashba-Edelstein effect in a two-dimensional electron gas: M. Yama, M. Matsuo and T. Kato, in: *Proceedings Volume 13119, Spintronics XVII* (SPIE, 2024), 105.

## Kawabata group

Recent years have seen remarkable progress in the physics of open quantum systems. In view of the recent rapid development of quantum information science and technology, it seems urgent to develop a general theory of open quantum systems. In our group, we are broadly interested in theoretical condensed matter physics, with a particular focus on nonequilibrium physics, to establish new foundations and principles in contemporary physics. Our recent research highlights topological phases of open quantum systems, as well as dissipative quantum chaos and lack thereof. On the basis of fundamental concepts such as symmetry and topology, we aim to uncover new physics intrinsic to far from equilibrium.

1. Topological enhancement of nonnormality in non-Hermitian skin effects: Y. O. Nakai, N. Okuma, D. Nakamura, K. Shimomura and M. Sato, *Phys. Rev. B* **109**, 144203 (2024).
2. Lieb-Schultz-Mattis Theorem in Open Quantum Systems: K. Kawabata, R. Sohal and S. Ryu, *Phys. Rev. Lett.* **132**, 070402 (2024).
3. Non-Hermitian Topology in Hermitian Topological Matter: S. Hamanaka, T. Yoshida and K. Kawabata, *Phys. Rev. Lett.* **133**, 266604 (2024).
4. Universal hard-edge statistics of non-Hermitian random matrices: Z. Xiao, R. Shindou and K. Kawabata, *Phys. Rev. Research* **6**, 023303 (2024).
5. Field theory of non-Hermitian disordered systems: Z. Chen, K. Kawabata, A. Kulkarni and S. Ryu, *Phys. Rev. B* **111**, 054203 (2025).
6. Multifractality of the many-body non-Hermitian skin effect: S. Hamanaka and K. Kawabata, *Phys. Rev. B* **111**, 035144 (2025).
7. Universal Stochastic Equations of Monitored Quantum Dynamics: Z. Xiao, T. Ohtsuki and K. Kawabata, *Phys. Rev. Lett.* **134**, 140401 (2025).
8. Non-linear sigma models for non-Hermitian random matrices in symmetry classes  $AI^\dagger$  and  $AIII^\dagger$ : A. Kulkarni, K. Kawabata and S. Ryu, *J. Phys. A* **58**, 225202 (2025).
9. Topological Order Intrinsic to Mixed Quantum States: K. Kawabata, *Physics* **18**, 9 (2025).

## Division of Nanoscale Science

### Otani group

In 2024, we made significant progress in spintronics, magnonics, and antiferromagnetic systems by developing new methods to control and detect spin, orbital, and phononic dynamics. We demonstrated enhanced magnetoacoustic coupling via spin current. We studied spin relaxation in monolayers and generated out-of-plane spin currents at ferromagnet/EuS interfaces. In antiferromagnets, we controlled chiral and octupole domain walls, observed fast domain-wall motion, and imaged cluster magnetic octupole moments in MnSn nanowires. We also achieved perpendicular magnetization in noncollinear systems. In magnonics, we demonstrated strong spin wave–SAW coupling, nonreciprocal magnetoacoustic waves, and hybrid magnon-phonon crystals. We tuned magnon-magnon interactions and examined underlayer effects in heterostructures. We applied these insights to high-sensitivity SAW magnetic sensors and contributed to broader perspectives through the 2024 magnonics roadmap and a chapter on voltage-controlled anisotropy. Together, we advanced low-power spintronic technologies through collaborative, cross-disciplinary research.

1. The 2024 magnonics roadmap: B. Flebus, D. Grundler, B. Rana, Y. Otani, I. Barsukov, A. Barman, G. Gubbiotti, P. Landeros, J. Akerman, U. Ebels, P. Pirro, V. E. Demidov, K. Schultheiss, G. Csaba, Q. Wang, F. Ciubotaru, D. E. Nikonov, P. Che, R. Hertel, T. Ono, D. Afanasiev, J. Mentink, T. Rasing, B. Hillebrands, S. V. Kusminskiy, W. Zhang, C. R. Du, A. Finco, T. van der Sar, Y. K. Luo, Y. Shiota, J. Sklenar, T. Yu and J. Rao, *J. Phys.: Condens. Matter* **36**, 363501 (2024).
2. Generation of out-of-plane polarized spin current in (permalloy, Cu)/EuS interfaces: P. Gupta, N. Chowdhury, M. Xu, P. K. Muduli, A. Kumar, K. Kondou, Y. Otani and P. K. Muduli, *Phys. Rev. B* **109**, L060405 (2024).
3. Role of the nonmagnetic underlayer in controlling the electronic structure of ferromagnet/nonmagnetic-metal heterostructures: D. Panda, K. K. Behera, S. Madhur, B. Rana, A. Gloskovskii, Y. Otani, A. Barman and I. Sarkar, *Phys. Rev. B* **110**, 094424 (2024).
4. Spin relaxation of localized electrons in monolayer MoSe<sub>2</sub>: Importance of random effective magnetic fields: E. Yalcin, I. V. Kalitukha, I. A. Akimov, V. L. Korenev, O. S. Ken, J. Puebla, Y. Otani, O. M. Hutchings, D. J. Gillard, A. I. Tartakovskii and M. Bayer, *Phys. Rev. B* **110**, L161405 (2024).

5. Observation of Cluster Magnetic Octupole Domains in the Antiferromagnetic Weyl Semimetal  $\text{Mn}_3\text{Sn}$  Nanowire: H. Isshiki, N. Budai, A. Kobayashi, R. Uesugi, T. Higo, S. Nakatsuji and Y. Otani, *Phys. Rev. Lett.* **132**, 216702 (2024).
6. Strongly Coupled Spin Waves and Surface Acoustic Waves at Room Temperature: Y. Hwang, J. Puebla, K. Kondou, C. Gonzalez-Ballester, H. Isshiki, C. S. Munoz, L. Liao, F. Chen, W. Luo, S. Maekawa and Y. Otani, *Phys. Rev. Lett.* **132**, 056704 (2024).
7. Nonreciprocal magnetoacoustic waves with out-of-plane phononic angular momenta: L. Liao, F. Chen, J. Puebla, J.-I. Kishine, K. Kondou, W. Luo, D. Zhao, Y. Zhang, Y. Ba and Y. Otani, *Sci. Adv.* **10**, eado2504 (2024).
8. Current-driven fast magnetic octupole domain-wall motion in noncollinear antiferromagnets: M. Wu, T. Chen, T. Nomoto, Y. Tserkovnyak, H. Isshiki, Y. Nakatani, T. Higo, T. Tomita, K. Kondou, R. Arita, S. Nakatsuji and Y. Otani, *Nat Commun* **15**, 4305 (2024).
9. Widen-dynamic-range surface acoustic wave magnetic sensors with high sensitivity: F. Chen, J. Lu, S. Liang, Y. Otani, X. Yang, Y. Zhang and W. Luo, *Journal of Alloys and Compounds* **980**, 173635 (2024).
10. Effect of the underlayer on the elastic parameters of the  $\text{CoFeB}/\text{MgO}$  heterostructures: S. Shekhar, S. Mielcarek, Y. Otani, B. Rana and A. Trzaskowska, *Scientific Reports* **14**, 20259 (2024).
11. Tunable strong magnon-magnon coupling in two-dimensional array of diamond shaped ferromagnetic nanodots: S. Majumder, S. Choudhury, S. Barman, Y. Otani and A. Barman, *Phys. Scr.* **99**, 025935 (2024).
12. Hybrid magnon-phonon crystals: L. Liao, J. Liu, J. Puebla and Q. S. & Y. Otani, *npj Spintronics* **3**, 6 (2024).
13. Selective Data Writing in IrMn-Based Perpendicular Magnetic Tunnel Junction Array Through Voltage-Gated Spin-Orbit Torque: W. Li, Z. Liu, S. Peng, J. Lu, J. Liu, X. Li, S. Lu, Y. Otani and W. Zhao, *IEEE Electron Device Lett.* **45**, 921 (2024).
14. Nonreciprocal resonant surface acoustic wave absorption in  $\text{Y}_3\text{Fe}_5\text{O}_{12}$ : Y. Ba, J. Puebla, K. Yamamoto, Y. Hwang, L. Liao, S. Maekawa, O. Klein and Y. Otani, *Phys. Rev. B* **111**, 104401 (2025).

## Hasegawa group

It is known that the vortices of monolayer superconductors formed on a substrate vary in shape at substrate steps because of the disruption of the electronic states. Vortices trapped at the steps on the striped incommensurate (SIC) phase of the Pb monolayer (ML) formed on a Si(111) substrate exhibited a round shape like those on the terraces. In contrast, the step-trapped vortices on the  $\sqrt{3} \times \sqrt{7}$  Pb ML phase are elongated along the step direction, which are called Josephson-Abrikosov vortices. From the different vortex shapes, one can expect different strengths of electronic decoupling in the steps. To directly observe the different decoupling, we performed scanning tunnelling potentiometry (STP), which enables us to obtain the electrochemical potential distribution with the same spatial resolution as scanning tunneling microscopy (STM). We performed STP on the two Pb ML phases and found clear potential drops at the  $\sqrt{3} \times \sqrt{7}$  Pb ML phase steps, whereas there was almost no drop in the SIC phase steps. This is the first quantitative demonstration of the resistivity of steps and their influence on superconductivity as a single disorder.

1.  $\dagger$ \*Quasi-Periodic Growth of One-Dimensional Copper Boride on Cu(110): Y. Tsujikawa, X. Zhang, K. Yamaguchi, M. Haze, T. Nakashima, A. Varadwaj, Y. Sato, M. Horio, Y. Hasegawa, F. Komori, M. Oshikawa, M. Kotsugi, Y. Ando, T. Kondo and I. Matsuda, *Nano Lett.* **24**, 1160 (2024).
2.  $\dagger$ \*Dimensional crossover and chirality of boron adsorbates on copper (110) surfaces: Y. Tsujikawa, T. Nakashima, X. Zhang, K. Yamaguchi, M. Horio, M. Haze, Y. Hasegawa, F. Komori, T. Kondo, Y. Ando and I. Matsuda, *Phys. Rev. Materials* **8**, 084003 1-7 (2024).
3.  $\dagger$ Bound states in the core of ordered vortices in stoichiometric iron-based superconductor  $\text{CaKFe}_4\text{As}_4$ : W. Wu, W. Li, Y. Chen, M. Haze, T. Tamegai and Y. Hasegawa, *Phys. Rev. B* **111**, 054510 1-9 (2025).
4. Simple Model for Striped-incommensurate Phase Formed by Pb Adsorption on Si(111): M. Yamada, Y. Sato, M. Haze and Y. Hasegawa, *e-J. Surf. Sci. Nanotechnol.* **23**, 2025-019 1-8 (2025).
5.  $\dagger$ Localized creation of bubble domains in  $\text{Fe}_3\text{GaTe}_2$  by conductive atomic force microscopy: C.-M. Liu, Y.-J. Liu, P.-C. Chang, P.-W. Chen, M. Haze, M.-H. Hsu, N. N. Gopakumar, Y. Zhou, Y.-H. Tung, S. Hammouda, C.-H. Du, Y. Hasegawa, Y. Su, H.-C. Chiu and W.-C. Lin, *Applied Surface Science Advances* **26**, 100718 1-8 (2025).

## Lippmaa group

Slightly canted, non-collinear antiferromagnets have very fast spin dynamics and the small residual magnetic moment can be used to probe the spin orientation and the domain structure that are normally difficult to quantify in antiferromagnetic materials. We are developing fabrication methods for obtaining high-quality antiferromagnetic films. The starting point is the orthoferrite  $\text{YFeO}_3$ , for which the magnetic domain structure can be controlled by the use of an orthorhombic substrate as an epitaxial template. This technique has allowed us to fabricate films large magnetic domains that have similar switching behavior to bulk single crystals, opening a path to developing thin-film-based magnetic switching devices.

1. \*Fabrication of single-crystalline  $\text{YFeO}_3$  films with large antiferromagnetic domains: C. Wang, M. Lippmaa and S. Nakatsuji, *J. Appl. Phys.* **135**, 113901 (1-8) (2024).
2. Polarity of homoepitaxial  $\text{ZnO}$  films grown by Nd:YAG pulsed laser deposition: T. Masuda, T. Sato, M. Lippmaa, T. Dazai, N. Sekine, I. Hosako, H. Koinuma and R. Takahashi, *J. Appl. Phys.* **136**, 095303 (1-8) (2024).
3. †The use of He buffer gas for moderating the plume kinetic energy during Nd:YAG-PLD growth of  $\text{Eu}_x\text{Y}_{2-x}\text{O}_3$  phosphor films: S. Suzuki, T. Dazai, T. Tokunaga, T. Yamamoto, R. Katoh, M. Lippmaa and R. Takahashi, *J. Appl. Phys.* **135**, 195302 (2024).
4. \*Broken Screw Rotational Symmetry in the Near-Surface Electronic Structure of *AB*-Stacked Crystals: H. Tanaka, S. Okazaki, M. Kobayashi, Y. Fukushima, Y. Arai, T. Iimori, M. Lippmaa, K. Yamagami, Y. Kotani, F. Komori, K. Kuroda, T. Sasagawa and T. Kondo, *Phys. Rev. Lett.* **132**, 136402 (1-6) (2024).

## Hashisaka group

We have continued setting up our experimental equipment, including introducing a dilution refrigerator. Alongside this, we conducted joint research on the on-chip transport of graphene plasmons and published review papers reporting on quantum transport in fractional quantum Hall systems. We also worked on developing nano-fabrication technology for quantum materials and creating nano-devices from candidate materials for quantum spin liquids, and we have already obtained some experimental results.

1. Gate-tunable giant superconducting nonreciprocal transport in few-layer  $\text{Td-MoTe}_2$ : T. Wakamura, M. Hashisaka, S. Hoshino, M. Bard, S. Okazaki, T. Sasagawa, T. Taniguchi, K. Watanabe, K. Muraki and N. Kumada, *Phys. Rev. Research* **6**, 013132 (2024).
2. エッジ状態のダイナミクスとエニオン統計: 橋坂 昌幸, 物性若手夏の学校テキスト **68**, 240 (2024).
3. On-chip transfer of ultrashort graphene plasmon wave packets using terahertz electronics: K. Yoshioka, G. Bernard, T. Wakamura, M. Hashisaka, K.-I. Sasaki, S. Sasaki, K. Watanabe, T. Taniguchi and N. Kumada, *Nat Electron* **7**, 537 (2024).
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5. Mach-Zehnder interference of fractionalized electron-spin excitations: T. Shimizu, E. Iyoda, S. Sasaki, A. Endo, S. Katsumoto, N. Kumada and M. Hashisaka, *Phys. Rev. B* **111**, L161406 (2025).
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## Yoshinobu group

We conducted several research projects in the fiscal year 2024: (1) The hydrogenation of formate and formaldehyde species on the  $\text{H-Cu}(997)$  surface was studied by HREELS and TPD. Several species were observed as desorption products by TPD, and intermediate species were identified. (2) The adsorption and decomposition of methanol on the  $\text{Cu}(977)$  and  $\text{Pd-Cu}(977)$  surfaces were studied by TPD, IRAS and SR-XPS, and selective dehydrogenation into formaldehyde was observed without oxygen. (3) The reactive desorption of  $\text{CO} + \text{O} \rightarrow \text{CO}_2$  on  $\text{Pt}(111)$  was studied using ab-initio molecular dynamics (AIMD) with van der Waals DFT functionals. The desorption dynamics of  $\text{CO}_2$  including kinetic energy, angular distribution and vibrational excitation were quantitatively elucidated. In addition, multidimensional neural network potential have been investigated. (4) The chemical states and reactions on the basal plane and the edge plane of  $\text{MoS}_2$  and HOPG were studied by SR-XPS. (5) SFG spectroscopy was developed using ultra-broadband terahertz and visible ultra-short pulse laser and applied to polymer films.

1. †Element-specific cluster growth on the two-dimensional metal-organic network: N. Tsukahara, R. Arafune and J. Yoshinobu, *Jpn. J. Appl. Phys.* **63**, 065504 (2024).

2. <sup>†</sup>\*Observation of Terahertz Spin Hall Conductivity Spectrum in GaAs with Optical Spin Injection: T. Fujimoto, T. Kurihara, Y. Murotani, T. Tamaya, N. Kanda, C. Kim, J. Yoshinobu, H. Akiyama, T. Kato and R. Matsunaga, Phys. Rev. Lett. **132**, 016301(1-7) (2024).
3. \*Ultra-broadband detection of coherent infrared pulses by sum-frequency generation spectroscopy in reflection geometry: R. Kameyama, S. Tanaka, Y. Murotani, T. Matsuda, N. Kanda, R. Matsunaga and J. Yoshinobu, Opt. Lett. **49**, 3978 (2024).
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11. \*Discovery of bicyclic borane molecule B<sub>14</sub>H<sub>26</sub>: X. Zhang, T. Fujino, Y. Ando, Y. Tsujikawa, T. Wang, T. Nakashima, H. Sakurai, K. Yamaguchi, M. Horio, H. Mori, J. Yoshinobu, T. Kondo and I. Matsuda, Commun Chem **8**, 14 (2025).
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15. 準大気圧光電子分光法による二酸化炭素水素化のオペランド観測: 小坂谷 貴典, 山本 達, 松田 巖, 吉信 淳, 横山 利彦, 表面と真空 **67**, 117-122 (2024).

## Functional Materials Group

### Akiyama group

In 2024, we demonstrated low power consumption of 0.5W and high output pulse-energy stability within 1% in our original ps gain-switched-LD seed-pulse prototype modules. In collaboration with Katayama-team in Yokohama National University, we started fs single-shot characterization of gain-switched pulses from the module. We analytically studied criteria of output gain in photovoltaic-thermoelectric tandems. Collaboration work and papers with Hiyama-team in Gunma University clarified inhibition sensitivity of in vitro firefly bioluminescence quantum yields to bivalent metal ion concentrations in aqueous solutions, and bioluminescence quantum yield of new luciferin analogs.

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11. \*Portable laser diode module of sub-10 ps gain-switched pulse source at 1030 nm wavelength: M. Kobayashi, H. Nakamae, C. Kim, T. Nakamura, T. Ito, S. Chen, Y. Kobayashi and H. Akiyama, *Jpn. J. Appl. Phys.* **64**, 038004 (2025).
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16. \*Structural Changes in the Retinal Chromophore and Ion-Conducting Pathway of an Anion Channelrhodopsin *GtACR1*: K. Shibata, Y. Kawasaki, S. Takaramoto, M. Watanabe, M. Fukuda, R. Ono, H. E. Kato, H. Akiyama and K. Inoue, *J. Phys. Chem. Lett.* **16**, published on the web (2025).
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20. †Inhibition sensitivity of *in vitro* firefly bioluminescence quantum yields to  $\text{Zn}^{2+}$  and  $\text{Cd}^{2+}$  concentrations in aqueous solutions: R. Ono, K. Saito, D. Tezuka, S. Yoshii, M. Kobayashi, H. Akiyama, N. Koga, H. Itabashi and M. Hiyama, *Photochem & Photobiology* **00**, php.14024 (2025).

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## Sugino group

The activity of this fiscal year includes computational study of materials using the first-principles density functional methods. Design of an electrochemical catalyst, elucidation of hydrogen diffusion on a metal surface, and analysis of magnetic properties of a cuprate. This group is also involved with cooperative work with experimental group, such as elucidation of CO dynamics on a metal surface, and analysis of muon in a Li-ion cathode material.

1. Magnetic phases of electron-doped infinite-layer  $\text{Sr}_{1-x}\text{La}_x\text{CuO}_2$  from first-principles density functional calculations: A. N. Tatan, J. Haruyama and O. Sugino, *Phys. Rev. B* **109**, 165134 (2024).
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4.  $^{\dagger}$ Elucidation of CO Oxidation and  $\text{CO}_2$  Desorption Dynamics on Pt(111) by van der Waals DFT Calculations: Hyperthermal Kinetic Energy, Sharp Desorption Angle, and Excited Vibrational States: H. Li, Y. Kataoka, S. Tanaka, J. Haruyama, O. Sugino and J. Yoshinobu, *J. Phys. Chem. C* **128**, 15393 (2024).
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## Oka group

Oka group has worked on Nonequilibrium quantum materials including Floquet engineering of Dirac semimetals, spin systems, and many-body systems.

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5. Floquet Weyl states at one-photon resonance: An origin of nonperturbative optical responses in three-dimensional materials: Y. Hirai, S. Okumura, N. Yoshikawa, T. Oka and R. Shimano, *Phys. Rev. Research* **6**, L012027-1-6 (2024).
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## Inoue group

In 2024, we identified a new family of anion-pumping rhodopsins, Glycylchlorhodopsin (GHR), from soil bacteria. This family is distinct from other anion-pumping rhodopsins and features a novel DTG motif in the third transmembrane helix, which includes a characteristic cytoplasmic glycine residue. X-ray crystallographic analysis revealed large cytoplasmic cavities formed due to the small size of this glycine residue. Time-resolved spectroscopic measurements demonstrated that the chloride release process through these cavities is distinct from that of canonical anion-pumping

rhodopsin from haloarchaea. Additionally, a new class of cation channel rhodopsin, HulaCCR, was identified through metatranscriptome analyses in Lake Hula in Israel. One member, HulaCCR1 exhibited non-specific cation transport, including the permeation of large cesium ions. Interestingly, truncation of either the N- or C-term extensions of HulaCCR1 altered its plasma membrane localization, indicating that the N- and C-termini play essential roles in determining cellular localization. Furthermore, we investigated the isomerization process of the retinal chromophore in inward proton-pumping schizorhodopsins, the quantum mechanical principles underlying the circular dichroic spectra of retinal chromophores in dimeric rhodopsins, and the ultrafast isomerization process in Archaerhodopsin-3 and its fluorescent variants, which hold promise for the development of genetically encoded voltage indicators.

1. \*Gilbert damping of NiFe thin films grown on two-dimensional chiral hybrid lead-iodide perovskites: T. Hatajiri, S. Sakamoto, H. Kosaki, Z. Tian, M. Tanaka, T. Ideue, K. Inoue, D. Miyajima and S. Miwa, Phys. Rev. B **110**, 054435 (1-6) (2024).
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## Hayashi group

In 2023, I moved to the Institute for Solid State Physics, and in 2024, three students participated in my lab. Together with a student, we wrote a review article on the application of extreme value analysis to axonal transport in neurons [Hayashi *et al.*, Biophys Rev 2024 ], based on our original research article published last year [Naoi *et al.*, Commun Phys 2024]. Regarding extreme value statistics, I also continued academic exchange with the Institute of Statistical Mathematic, and contributed to the joint research report “Applications of Extreme Value Theory to Engineering”, published by the Institute [Hayashi, the Institute of Statistical Mathematic Report 478, 2024].

Apart from extreme value analysis research activities, a particularly significant event in 2024 was the 21st Congress of the International Union for Pure and Applied Biophysics (IUPAB) held in Kyoto. I contributed as a member of the Executive Committee. I had been involved with the committee since 2017, when Japan successfully won the bid to host the congress, and thus completed a major responsibility. At the IUPAB Congress, I also served as the chair of the "Application of Non-equilibrium Physics" session [Hayashi and Li, *Biophys Rev* 2024]. As a member of the Executive Committee, I was in charge of the IUPAB Hands-on Training Program, and in collaboration with six universities and research institutes across Japan, we hosted approximately 70 early-career researchers from both Japan and abroad, who participated in the congress [Hayashi, *BPPB* 2024]. In addition, I participated in a roundtable discussion at IUPAB with promising researchers from Japan and abroad who had come to Japan for the congress, where we discussed the theme: "Dreaming the Next 50 Years in Our Biophysics" [Hayashi *et al.*, *BPPB* 2025]. In 2024, I was actively involved in various initiatives related to the organization of IUPAB. Through these efforts, I believe I was able to enhance the presence of the Institute for Solid State Physics in the Biophysical Society of Japan.

In addition, I was invited as a lecturer to the 69th Condensed Matter Physics Summer School for Young Researchers, where I led a seminar and interacted with Japanese students who study soft matter and non-equilibrium statistical mechanics. Since the Institute for Solid State Physics has supported this summer school, I was glad to have had the opportunity to contribute [Hayashi, *Lecture notes for the 69th Condensed Matter Physics Summer School*, 2025].

1. Extreme Value Analysis of Intracellular Cargo Transport by Motor Proteins: T. Naoi, Y. Kagawai, K. Nagino, S. Niwa and K. Hayashi, *Communications Physics* **7**, Article number: 50 (2024).
2. Commentary to "Application of Non-equilibrium Physics": a session of the 21st IUPAB Congress 2024, Kyoto, Japan: K. Hayashi and C.-B. Li, *Biophys Rev NA*, NA (2024).
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4. IUPAB 京都 2024 年会議における座談会：我々の生物物理学の次の 50 年を夢見て（前半）：林 久美子, G. HUMMER, J. A. JOSEPH, R. LI, 永井 健治, 大浪 修一, F. ZHANG, 北村 朗, 富樫 祐一, 角五 彰, 藤原 郁子, 小松崎 民樹, *生物物理* **65**, 35-46 (2025).
5. A round table at IUPAB Congress in Kyoto 2024: Dreaming the next 50 years in our biophysics: K. Hayashi, G. Hummer, J. A. Joseph, R. Li, T. Nagai, S. Onami, F. Zhang, A. Kitamura, Y. Togashi, A. Kakugo, I. Fujiwara and T. Komatsuzaki, *Biophysics and Physicobiology* **21**, NA (2025).
6. 極値統計解析の神経細胞軸索輸送への応用: 林久美子, 「統計数理研究所共同研究リポート 478 極値理論の工学への応用」 (統計数理研究所, 2025), 36-40.
7. Extreme-value analysis in nano-biological systems: applications and implications: K. Hayashi, N. Takamatsu and S. Takaramoto, *Biophys. Rev.* **16**, 571-579 (2024).
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## Quantum Materials Group

### Oshikawa group

We developed the finite-size scaling theory of one-dimensional quantum critical systems in the presence of boundaries. While the finite-size spectrum in the conformal limit, namely of a conformal field theory with conformally invariant boundary conditions, is related to the dimensions of boundary operators by Cardy, the actual spectra of lattice models are affected by both bulk and boundary perturbations and contain non-universal boundary energies. We obtain a general expression of the finite-size energy levels in the presence of bulk and boundary perturbations. In particular, a generic boundary perturbation related to the energy-momentum tensor gives rise to a renormalization of the effective system size. We verify our field-theory formulation by comparing the results with the exact solution of the critical transverse-field Ising chain and with accurate numerical results on the critical three-state Potts chain obtained by Density-Matrix Renormalization Group. Our study greatly improves the precision, and will serve as a basis of future numerical and analytical studies of boundary critical phenomena.

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2. <sup>†</sup>Intrinsic symmetry-protected topological mixed state from modulated symmetries and hierarchical structure of boundary anomaly: Y. You and M. Oshikawa, *Phys. Rev. B* **110**, 165160 (2024).
3. <sup>†</sup>Magnetization oscillations in a periodically driven transverse field Ising chain: X. Wang, M. Oshikawa, M. Kormos and J. Wu, *Phys. Rev. B* **110**, 195101 (2024).

4. †Spontaneous strong symmetry breaking in open systems: Purification perspective: P. Sala, S. Gopalakrishnan, M. Oshikawa and Y. You, *Phys. Rev. B* **110**, 155150 (2024).
5. †System-environment entanglement phase transitions: Y. Ashida, S. Furukawa and M. Oshikawa, *Phys. Rev. B* **110**, 094404 (2024).
6. †Lieb-Schultz-Mattis Theorem for 1D Quantum Magnets with Antiunitary Translation and Inversion Symmetries: Y. Yao, L. Li, M. Oshikawa and C.-T. Hsieh, *Phys. Rev. Lett.* **133**, 136705 (2024).
7. †\*Quasi-Periodic Growth of One-Dimensional Copper Boride on Cu(110): Y. Tsujikawa, X. Zhang, K. Yamaguchi, M. Haze, T. Nakashima, A. Varadwaj, Y. Sato, M. Horio, Y. Hasegawa, F. Komori, M. Oshikawa, M. Kotsugi, Y. Ando, T. Kondo and I. Matsuda, *Nano Lett.* **24**, 1160 (2024).
8. †Decorated defect construction of gapless-SPT states: L. Li, M. Oshikawa and Y. Zheng, *SciPost Phys.* **17**, 013 (2024).
9. Finite-size corrections to the energy spectra of gapless one-dimensional systems in the presence of boundaries: Y. Liu, H. Shimizu, A. Ueda and M. Oshikawa, *SciPost Phys.* **17**, 099 (2024).
10. †Entanglement swapping in critical quantum spin chains: M. Hoshino, M. Oshikawa and Y. Ashida, *Phys. Rev. B* **111**, 155143 (2025).
11. Self-congruent point in critical matrix product states: An effective field theory for finite-entanglement scaling: J. T. Schneider, A. Ueda, Y. Liu, A. Läuchli, M. Oshikawa and L. Tagliacozzo, *SciPost Phys.* **18**, 142 (2025).

## Nakatsuji group

Our research group is advancing a new phase in quantum materials science, where fundamental discoveries are increasingly connected with emerging quantum technologies through interdisciplinary collaboration. We focus on designing, synthesizing, and characterizing quantum materials that exhibit novel macroscopic properties. These materials are integrated into thin-film-based devices, enabling us to probe novel quantum functionalities and assess their technological potential. By forging direct links between quantum phenomena and practical applications, our mission is to lead the creation of material platforms that drive both scientific discovery and innovation in computing, sensing, and energy-saving technologies. Our major research themes are: 1. Quantum transport in magnetic topological materials 2. Coherent quantum spin transport in antiferromagnetic spintronics 3. Strange metal and exotic superconductivity in strongly correlated electron systems

1. \*Fabrication of single-crystalline YFeO<sub>3</sub> films with large antiferromagnetic domains: C. Wang, M. Lippmaa and S. Nakatsuji, *J. Appl. Phys.* **135**, 113901 (1-8) (2024).
2. \*Bulk and surface uniformity of magnetic and electronic structures in epitaxial W/Mn<sub>3</sub>Sn/MgO films revealed by fluorescence- and electron-yield x-ray magnetic circular dichroism: S. Sakamoto, T. Higo, Y. Kotani, H. Kosaki, T. Nakamura, S. Nakatsuji and S. Miwa, *Phys. Rev. B* **110**, L060412 (2024).
3. †\*Crystal field magnetostriction of spin ice under ultrahigh magnetic fields: N. Tang, M. Gen, M. Rotter, H. Man, K. Matsuhira, A. Matsuo, K. Kindo, A. Ikeda, Y. H. Matsuda, P. Gegenwart, S. Nakatsuji and Y. Kohama, *Phys. Rev. B* **110**, 214414 (1-10) (2024).
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5. \*Tunneling magnetoresistance and spin-orbit torque magnetization switching in ferrimagnetic Gd-Fe-Co based magnetic tunnel junction: M. Yunokizaki, Y. Hibino, H. Idzuchi, H. Tsai, M. Ishibashi, S. Miwa, M. Hayashi and S. Nakatsuji, *Jpn. J. Appl. Phys.* **64**, 010904 (2025).
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## Miwa group

This year we worked on the following topics: (1) chirality-induced spin selectivity (CISS) in the absence of charge current, (2) X-ray spectroscopy on the chiral antiferromagnet  $\text{Mn}_3\text{Sn}$  thin film, and (3) interfacial magnetic anisotropy of the Fe/LiF/MgO system. In topic (1), we have applied the spin-pumping method to the CISS experimental system and find that the CISS-induced magnetoresistance does not originate from the spin-dependent transport (Phys. Rev. B **110**, 054435). In topic (2), we find that our epitaxial  $\text{Mn}_3\text{Sn}$  thin film exhibits uniformity of magnetic and electronic states throughout the thickness region. This is a collaboration with the groups of Nakatsuji (Phys. Rev. B **110**, L060412). In topic (3) we find that alkali fluoride with good crystallinity is effective to enhance the perpendicular magnetic anisotropy of the Fe/MgO system (Phys. Rev. B **109**, 064413).

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5. \*Tunneling magnetoresistance and spin-orbit torque magnetization switching in ferrimagnetic Gd-Fe-Co based magnetic tunnel junction: M. Yunokizaki, Y. Hibino, H. Idzuchi, H. Tsai, M. Ishibashi, S. Miwa, M. Hayashi and S. Nakatsuji, Jpn. J. Appl. Phys. **64**, 010904 (2025).
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## Materials Design and Characterization Laboratory

### Hiroi group

We concentrate on the layered polyanionic material  $\text{MAIX}$  ( $M = \text{K}, \text{Na}$ ,  $X = \text{Si}, \text{Ge}$ ). This material is a type of intermetallic compound known as the Zintl phase, which has an unusual bonding state between ions and metals. Its electronic structure is distinguished by its nodal-line semimetal composition. This is a topological semimetal, consisting of a linear chain of Dirac points with linearly intersecting bands in wavenumber space (upper right in the figure), and is thought to have a nontrivial quantum state. We conducted various measurements on these materials and discovered that  $\text{NaAlSi}$  is a superconductor at 6.8 K,  $\text{NaAlGe}$  is an insulator with a pseudogap of approximately 100 K, and  $\text{KAlGe}$  undergoes a metal-metal transition at 89 K. Thus, elemental substitution produces a wide range of ground states, including the low-temperature phase of  $\text{KAlGe}$ , which has a remarkably low carrier density and extremely high mobility. Synchrotron X-ray diffraction experiments have revealed that microstructural changes accompanying the superlattice occur during this transition, resulting in the formation of Al-Ge tetramer "molecule formation". He has recently observed Fermi surfaces using angle-resolved photoemission spectroscopy, quasiparticle interferograms and topological edge states with STM, and structural phase transitions under high pressure.

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### Kawashima group

We developed efficient methods, algorithms, parallelized programs, and sometimes new concepts, based on novel numerical techniques such as the tensor network (TN) method and quantum Monte Carlo (QMC). We then applied them to relevant physical problems. To list subjects of our research in 2024: (1) Classical spin systems and novel phase transitions

and excitations [Akamatsu and Kawashima, JStatPhys191; Wu. et al. Phys. Rev. Res. 6], (2) Dynamics of quantum spin systems [Tu et al. PRXQuantum5], (3) Development of new tensor network methods [Homma, et al. Phys. Rev. Res. 6], and (4) Development of open-source software for condensed matter calculations [Ido, et al., Comp.Phys.Commun.298; Aoyama et al., Comp. Phys. Commun. 298]

1.  $\dagger$ \*H-wave – A Python package for the Hartree-Fock approximation and the random phase approximation: T. Aoyama, K. Yoshimi, K. Ido, Y. Motoyama, T. Kawamura, T. Misawa, T. Kato and A. Kobayashi, Computer Physics Communications **298**, 109087(1-10) (2024).
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4. Faithfulness of Real-Space Renormalization Group Maps: K. O. Akamatsu and N. Kawashima, J Stat Phys **191**, 109 (2024).
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8. Multi-impurity method for the bond-weighted tensor renormalization group: S. Morita and N. Kawashima, Phys. Rev. B **111**, 054433 (2025).
9. Tensor network renormalization approach to antiferromagnetic 6-state clock model on the Union Jack lattice: K. Homma, S. Morita and N. Kawashima, Phys. Rev. B **111**, 134427(1-12) (2025).

## Uwatoko group

1. Field-Induced Criticality in YbCu<sub>4</sub>Au: T. Taniguchi, K. Osato, H. Okabe, T. Kitazawa, M. Kawamata, S. Hashimoto, Y. Ikeda, Y. Nambu, D. P. Sari, I. Watanabe, J. G. Nakamura, A. Koda, J. Gouchi, Y. Uwatoko, S. Kittaka, T. Sakakibara, M. Mizumaki, N. Kawamura, T. Yamanaka, K. Hiraki, T. Sasaki and M. Fujita, J. Phys. Soc. Jpn. **93**, 124706(1-8) (2024).
2. \*Field-Induced Quantum Phase Transitions in the Pressure-Tuned Triangular-Lattice Antiferromagnet CsCuCl<sub>3</sub>: K. Nihongi, T. Kida, D. Yamamoto, Y. Narumi, J. Zaccaro, Y. Kousaka, K. Inoue, Y. Uwatoko, K. Kindo and M. Hagiwara, J. Phys. Soc. Jpn. **93**, 084704(1-7) (2024).
3. Pressure-induced Superconductivity in BiS<sub>2</sub>-based Superconductors Eu<sub>2</sub>SrBi<sub>2</sub>S<sub>2.5</sub>Se<sub>1.5</sub>F<sub>4</sub>: K. Ishigaki, J. Gouchi, K. Torizuka, S. Arumugam, A. K. Ganguli, Z. Haque, K. Ganesan, G. S. Thakur and Y. Uwatoko, J. Phys. Soc. Jpn. **93**, 024706(1-4) (2024).
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8. Quantum criticality in YbCu<sub>4</sub>Ni: K. Osato, T. Taniguchi, H. Okabe, T. Kitazawa, M. Kawamata, Z. Hongfei, Y. Ikeda, Y. Nambu, D. P. Sari, I. Watanabe, J. G. Nakamura, A. Koda, J. Gouchi, Y. Uwatoko and M. Fujita, Phys. Rev. B **109**, 024435(1-6) (2024).

9. \*Bulk high-temperature superconductivity in pressurized tetragonal  $\text{La}_2\text{PrNi}_2\text{O}_7$ : N. Wang, G. Wang, X. Shen, J. Hou, J. Luo, X. Ma, H. Yang, L. Shi, J. Dou, J. Feng, J. Yang, Y. Shi, Z. Ren, H. Ma, P. Yang, Z. Liu, Y. Liu, H. Zhang, X. Dong, Y. Wang, K. Jiang, J. Hu, S. Nagasaki, K. Kitagawa, S. Calder, J. Yan, J. Sun, B. Wang, R. Zhou, Y. Uwatoko and J. Cheng, *Nature* **634**, 579-584 (2024).
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## Ozaki group

A noniterative method is presented to calculate the closest Wannier functions (CWFs) to a given set of localized guiding functions, such as atomic orbitals, hybrid atomic orbitals, and molecular orbitals, based on minimization of a distance measure function. It is shown that the minimization is directly achieved by a polar decomposition of a projection matrix via singular value decomposition, making iterative calculations and complications arising from the choice of the gauge irrelevant. The disentanglement of bands is inherently addressed by introducing a smoothly varying window function and a greater number of Bloch functions, even for isolated bands. In addition to atomic and hybrid atomic orbitals, we introduce embedded molecular orbitals in molecules and bulks as the guiding functions, and demonstrate that the Wannier interpolated bands accurately reproduce the targeted conventional bands of a wide variety of systems including Si, Cu, the TTF-TCNQ molecular crystal, and a topological insulator of  $\text{Bi}_2\text{Se}_3$ . We further show the usefulness of the proposed method for calculating effective atomic charges. These numerical results not only establish our proposed method as an efficient alternative for calculating WFs, but also suggest that the concept of CWF can serve as a foundation for developing novel methods to analyze electronic structures and calculate physical properties.

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10. Dimer ribbon structures on diamond (001) surfaces revealed with atomic force microscopy: R. Zhang, Y. Yasui, M. Fukuda, M. Ogura, T. Makino, D. Takeuchi, T. Ozaki and Y. Sugimoto, *Phys. Rev. Research* **7**, 023036 (2025).

## Noguchi group

We have studied (1) spatiotemporal patterns in active Potts models, (2) curvature sensing of asymmetric proteins and rotationally symmetric proteins, and (3) dynamics of tissue sheets on substrates.

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2. Curvature sensing of curvature-inducing proteins with internal structure: H. Noguchi, *Phys. Rev. E* **109**, 024403/1-10 (2024).
3. Growth and shrinkage of tissue sheets on substrates: buds, buckles, and pores: H. Noguchi and J. Elgeti, *New J. Phys.* **26**, 103027 (2024).
4. Spatiotemporal patterns in the active cyclic Potts model: H. Noguchi and J.-B. Fournier, *New J. Phys.* **26**, 093043 (2024).
5. Spontaneous symmetry breaking in two dimensions under non-equilibrium laminar flows: Y. Minami and H. Nakano, *J. Stat. Mech.* **2024**, 113205 (2024).
6. Computer Simulations of Responsive Nanogels at Lipid Membrane: A. S. Sorokina, R. A. Gumerov, H. Noguchi and I. I. Potemkin, *Macromol. Rapid Commun.* **45**, 2400406 (2024).
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11. Spatiotemporal patterns in active four-state Potts models: H. Noguchi, *Sci Rep* **15**, 674 (2025).
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## Yoshimi group

In 2024, we continued our contributions to the Project for Advancement of Software Usability in Materials Science (PASUMS) by developing and maintaining research software tools. One of our main developments was ODAT-SE (Open Data Analysis Tool for Science and Engineering), a general-purpose data analysis platform that integrates forward problem solvers with inverse problem-solving algorithms for optimization tasks. Formerly known as 2DMAT, ODAT-SE was restructured in version 3 with a modular architecture to enhance applicability across various scientific domains. We also extended the capabilities of DCore and developed ChiQ, a new tool for computing two-particle spectra from DMFT results. In parallel with software development, we conducted theoretical studies on pressure-induced electronic structure changes in organic conductors, including investigations of Fermi surface topology, phase transitions, and orbital hybridization effects on conductivity. Furthermore, we collaborated on experimental data analysis projects involving coherent X-ray diffraction and spectro-ptychography, applying machine learning techniques.

1. †Multipolar ordering from dynamical mean field theory with application to CeB<sub>6</sub>: J. Otsuki, K. Yoshimi, H. Shinaoka and H. O. Jeschke, *Phys. Rev. B* **110**, 035104 (2024).
2. †\*Compensated Ferrimagnets with Colossal Spin Splitting in Organic Compounds: T. Kawamura, K. Yoshimi, K. Hashimoto, A. Kobayashi and T. Misawa, *Phys. Rev. Lett.* **132**, 156502(1-6) (2024).
3. †\*Sub-photon accuracy noise reduction of a single shot coherent diffraction pattern with an atomic model trained autoencoder: T. Ishikawa, Y. Takeo, K. Sakurai, K. Yoshinaga, N. Furuya, Y. Inubushi, K. Tono, Y. Joti, M. Yabashi, T. Kimura and K. Yoshimi, *Opt. Express* **32**, 18301 (2024).
4. †\*H-wave – A Python package for the Hartree-Fock approximation and the random phase approximation: T. Aoyama, K. Yoshimi, K. Ido, Y. Motoyama, T. Kawamura, T. Misawa, T. Kato and A. Kobayashi, *Computer Physics Communications* **298**, 109087(1-10) (2024).
5. †\*Orbital hybridization of donor and acceptor to enhance the conductivity of mixed-stack complexes: T. Fujino, R. Kameyama, K. Onozuka, K. Matsuo, S. Dekura, T. Miyamoto, Z. Guo, H. Okamoto, T. Nakamura, K. Yoshimi, S. Kitou, T.-H. Arima, H. Sato, K. Yamamoto, A. Takahashi, H. Sawa, Y. Nakamura and H. Mori, *Nat Commun* **15**, 3028 (2024).
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7. †\*Update of HΦ : Newly added functions and methods in versions 2 and 3: K. Ido, M. Kawamura, Y. Motoyama, K. Yoshimi, Y. Yamaji, S. Todo, N. Kawashima and T. Misawa, *Comp. Phys. Commun.* **298**, 109093(1-15) (2024).
8. \*Pressure-induced topological changes in the Fermi surface of a two-dimensional molecular conductor: T. Kobayashi, K. Yoshimi, H. Ma, S. Sekine, H. Taniguchi, N. Matsunaga, A. Kawamoto and Y. Uwatoko, *Phys. Rev. Materials* **9**, L021801(1-8) (2025).

## Okamoto group

The discovery of a new material has a potential to trigger the evolution of condensed matter physics. We aim at discovering new materials of crystalline solids that exhibit novel quantum phenomena and innovative electronic functions. In this year, we reported the results of our research on new superconductors Zr<sub>6</sub>RuBi<sub>2</sub> and Zr<sub>6</sub>FeBi<sub>2</sub> and new quasi-one-dimensional van der Waals crystal Ta<sub>2</sub>Ni<sub>3</sub>Te<sub>5</sub>. The A<sub>6</sub>MX<sub>2</sub> family with the hexagonal Zr<sub>6</sub>CoAl<sub>2</sub>-type structure is a hotspot for exploring new *d*-electron superconductors, in which ten new superconductors have been discovered in the past year. The highest  $T_c = 4.7$  K is manifested in Sc<sub>6</sub>FeTe<sub>2</sub>, where the contribution of the Fe 3*d* orbitals is considerably large, indicating that A<sub>6</sub>MX<sub>2</sub> can be a potential target for studying the correlation between superconductivity and various features of transition metals. In this year, we discovered the two new bulk superconductors Zr<sub>6</sub>RuBi<sub>2</sub> and Zr<sub>6</sub>FeBi<sub>2</sub> with  $T_c = 4.9$  and 1.4 K, respectively. The former compound is a new material and its  $T_c$  is slightly higher than that of Sc<sub>6</sub>FeTe<sub>2</sub>, highest in the existing A<sub>6</sub>MX<sub>2</sub> compounds. Based on the electrical resistivity, magnetization, and heat capacity data, the superconductivity in Zr<sub>6</sub>RuBi<sub>2</sub> is found to be most likely a conventional BCS type, but the considerably higher  $T_c$  than that for Zr<sub>6</sub>FeBi<sub>2</sub> differs from the trend in the other A<sub>6</sub>MX<sub>2</sub> superconductors, suggesting the high potential of A<sub>6</sub>MX<sub>2</sub> family to realize higher  $T_c$  and unusual properties. We succeeded in synthesizing the single crystals of chemically doped Ta<sub>2</sub>Ni<sub>3</sub>Te<sub>5</sub>. Cr-doped Ta<sub>2</sub>Ni<sub>3</sub>Te<sub>5</sub> was found to show high thermoelectric performance, in which the telluride with the one-dimensional crystal structure plays an important role.

1. Superconductivity in Ternary Germanide ScPdGe and Silicide ScPdSi: Y. Shinoda, Y. Okamoto, Y. Yamakawa, H. Takatsu, H. Kageyama, D. Hirai and K. Takenaka, *J. Phys. Soc. Jpn.* **93**, 023701(1-4) (2024).
2. Superconductivity in Ternary Zirconium Telluride Zr<sub>6</sub>MTe<sub>2</sub> with 3d Transition Metals: H. Matsumoto, Y. Yamakawa, R. Okuma, D. Nishio-Hamane and Y. Okamoto, *J. Phys. Soc. Jpn.* **93**, 023705(1-5) (2024).

3. †Anisotropic Optical Conductivity Accompanied by a Small Energy Gap in One-Dimensional Thermoelectric Telluride Ta<sub>4</sub>SiTe<sub>4</sub>: F. Matsunaga, Y. Okamoto, Y. Yokoyama, K. Takehana, Y. Imanaka, Y. Nakamura, H. Kishida, S. Kawano, K. Matsuhira and K. Takenaka, Phys. Rev. B **109**, L161105(1-6) (2024).
4. 1次元ファンデルワールス結晶 Ta<sub>4</sub>SiTe<sub>4</sub> における熱電効果: 岡本 佳比古, 山川 洋一, 竹中 康司, 固体物理 **59**, 95-105 (2024).
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6. Electric Field-Induced Volume Change in Pyro-Vanadate-Phosphates: Toward an Alternative Actuator Architecture: K. Takada, J. Shibutani, K. Yagi, F. Ikawa, Y. Yokoyama, D. Hirai, Y. Okamoto, N. Katayama, Y. Uemura, L. M. G. H. Chavas, T. Hatano, A. Fujita and K. Takenaka, Appl. Phys. Lett. **125**, 041903(1-6) (2024).
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8. Unbalanced Charge Distribution Stabilized by Orbital Ordering: Y. Okamoto, JPSJ News and Comments **21**, 13(1-2) (2024).
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11. Anisotropic superconducting gap probed by Te<sup>125</sup> NMR in noncentrosymmetric Sc<sub>6</sub>MTe<sub>2</sub> (M = Fe, Co): K. Doi, H. Takei, Y. Shinoda, Y. Okamoto, D. Hirai, K. Takenaka, T. Matsushita, Y. Kobayashi and Y. Shimizu, Phys. Rev. B **111**, 214502(1-7) (2025).
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15. \*Topological Semimetal KAlGe with Novel Electronic Instability: T. Ikenobe, T. Yamada, J.-I. Yamaura, T. Oguchi, R. Okuma, D. Hirai, H. Sagayama, Y. Okamoto and Z. Hiroi, Chem. Mater. **37**, 189-197 (2025).
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## Yamaura group

This year, the structures of numerous materials were elucidated utilizing quantum beams and laboratory-based diffractometers for fundamental to advanced materials such as innovative ferroelectrics, high dielectrics, unique thermoelectric materials, boron crystals, and nanowire sensors. The collaborative research in the X-ray diffraction section of the Materials Design and Characterisation Laboratory (MDCL) advanced effectively, offering user support to numerous individuals both within and beyond the laboratory, as well as analytical guidance, innovative research proposals, and avenues for quantum beam applications. In addition, the radiation safety laboratory was operated to educate and control radiation workers at the facility, control nuclear fuel materials, and conduct periodic inspections of X-ray generators.

1. Symmetry change in LaNiO<sub>3</sub> films caused by epitaxial strain from LaAlO<sub>3</sub>, SrTiO<sub>3</sub>, and DyScO<sub>3</sub> pseudocubic (001) surfaces: F. Izumisawa, Y. Ishii, M. Kimura, T. Katase, T. Kamiya, J.-I. Yamaura and Y. Wakabayashi, J. Appl. Phys. **136**, 075303 (2024).
2. \* $J_{eff} = 1/2$  Hyperoctagon Lattice in Cobalt Oxalate Metal-Organic Framework: H. Ishikawa, S. Imajo, H. Takeda, M. Kakegawa, M. Yamashita, J.-I. Yamaura and K. Kindo, Phys. Rev. Lett. **132**, 156702 (2024).
3. Phonon drag thermopower persisting over 200 K in FeSb<sub>2</sub> thin film on SrTiO<sub>3</sub> single crystal: C. Yamamoto, X. He, K. Hanzawa, T. Katase, M. Sasase, J.-I. Yamaura, H. Hiramatsu, H. Hosono and T. Kamiya, Appl. Phys. Lett. **124**, 193902 (2024).

4. <sup>†</sup>\*Crystal structure and properties of perovskite-type rubidium niobate, a high-pressure phase of RbNbO<sub>3</sub>: A. Yamamoto, K. Murase, T. Sato, K. Sugiyama, T. Kawamata, Y. Inaguma, J.-I. Yamaura, K. Shitara, R. Yokoi and H. Moriwake, Dalton Trans. **53**, 7044 (2024).
5. \*Macroscopic sheets of hydrogen boride and their spectroscopic evaluation: K. Yamaguchi, M. Niibe, X. Zhang, T. Sumi, M. Horio, Y. Ando, J.-I. Yamaura, E. Nakamura, K. Tanaka, T. Kondo and I. Matsuda, Phys. Rev. Materials **8**, 074005 (2024).
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9. <sup>†</sup>Dielectric properties depend on the crystal structure of perovskite-type RbTaO<sub>3</sub> synthesized at high pressure: K. Murase, J.-I. Yamaura, Y. Hamasaki, T. Kato, H. Sagayama and A. Yamamoto, Dalton Trans. **54**, 2252 (2025).
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11. Nano-Patterned CuO Nanowire Nanogap Hydrogen Gas Sensor with Voids: M. Zhao, R. Nitta, S. Izawa, J. Yamaura and Y. Majima, Adv Funct Materials **35**, 2415971 (2025).

## Kitagawa group

Kitagawa lab. started in FY2024. We are developing state-of-the-art high-pressure measurement techniques including quantum sensing, and exploring new phenomena under pressure. Our main targets in FY2024 included, nickelate high-temperature superconductors, and instrumental development of ultrahigh-pressure devices for SQUID magnetometry and optically-detected magnetic resonance (ODMR).

We established bulkiness of superconductivity for high-temperature two-layer-type nickelate superconductors for the first time. The nickelate superconductor was first discovered as a resistivity drop under pressure as high as 14 GPa in 2023, but there has been controversy whether the superconductivity is real (bulk) or not. We successfully measured Meissner effect using 6-8 multi anvil apparatus and conventional micro-coil mutual inductance method.

To accelerate research for novel superconductors or magnetic materials, we are developing two types of opposed-anvil type pressure devices. One fits to magnetization measurement using a commercial SQUID magnetometer, which allows a highly sensitive magnetometry with a resolution of volume susceptibility as small as  $10^{-3}$  under very high pressures up to 20 GPa. The other is a large-scale high-pressure system intended to be used with wide field-of-view ODMR of diamond NV center or other solid-state quantum sensors. We are now testing these technologies with pressure-induced superconductors including nickelates.

1. \*Bulk high-temperature superconductivity in pressurized tetragonal La<sub>2</sub>PrNi<sub>2</sub>O<sub>7</sub>: N. Wang, G. Wang, X. Shen, J. Hou, J. Luo, X. Ma, H. Yang, L. Shi, J. Dou, J. Feng, J. Yang, Y. Shi, Z. Ren, H. Ma, P. Yang, Z. Liu, Y. Liu, H. Zhang, X. Dong, Y. Wang, K. Jiang, J. Hu, S. Nagasaki, K. Kitagawa, S. Calder, J. Yan, J. Sun, B. Wang, R. Zhou, Y. Uwatoko and J. Cheng, Nature **634**, 579-584 (2024).

## Materials Synthesis and Characterization group

1. \* $J_{eff} = 1/2$  Hyperoctagon Lattice in Cobalt Oxalate Metal-Organic Framework: H. Ishikawa, S. Imajo, H. Takeda, M. Kakegawa, M. Yamashita, J.-I. Yamaura and K. Kindo, Phys. Rev. Lett. **132**, 156702 (2024).
2. <sup>†</sup>\*Crystal structure and properties of perovskite-type rubidium niobate, a high-pressure phase of RbNbO<sub>3</sub>: A. Yamamoto, K. Murase, T. Sato, K. Sugiyama, T. Kawamata, Y. Inaguma, J.-I. Yamaura, K. Shitara, R. Yokoi and H. Moriwake, Dalton Trans. **53**, 7044 (2024).

# Neutron Science Laboratory

## Yamamuro group

Our laboratory is studying chemical physics of complex condensed matters by using neutron scattering, X-ray diffraction, calorimetric, dielectric, and viscoelastic techniques. Our target materials are glasses, liquids, and various disordered solids. In 2024, we measured X-ray diffraction of hydrogen (H<sub>2</sub>) and xenon (Xe) amorphous hydrates M-5.75H<sub>2</sub>O (M: guest molecule) using a custom-made vapor-deposition cryostat and a high-energy X-ray diffractometer at BL04B2, SPring-8. We found that both amorphous hydrates had many distorted hydrogen-bonded H<sub>2</sub>O cages containing guest molecules, and they became more well-defined by annealing below  $T_g$  (= 130 K). It was also clarified that amorphous Xe hydrate transformed to crystalline Xe hydrate by annealing around 165 K. We performed the neutron powder diffraction (NPD) and quasielastic neutron scattering (QENS) experiments on a new hydrogen cluster material Mg<sub>6</sub>WH<sub>16</sub>. The orientation of the MoH<sub>8</sub><sup>4+</sup> ions remain disordered down to 8 K and the QENS spectra were well fitted by the Kohlrausch-Williams-Watts (KWW) functions with small non-exponential parameters ( $\beta < 0.4$ ) corresponding to large distribution of relaxation time. The heat capacities of vapor-deposited amorphous H<sub>2</sub>O and CS<sub>2</sub> were measured to obtain absolute density of states corresponding to boson peaks. We also measured the heat capacity of a metal-organic framework MOF-101 including acetonitrile (AN) molecules with/without Mg(TFSI)<sub>2</sub> in the pores to investigate the states of AN molecules from an entropic point of view.

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3. Non-Newtonian Dynamics in Water-in-Salt Electrolytes: T. Yamaguchi, A. Dukhin, Y. -J. Ryu, D. Zhang, O. Borodin, M. A. Gonza'lez, O. Yamamuro, D. L. Price and M. -L. Saboungi, *J. Phys. Chem. Lett.* **15**, 76-80 (2024).
4. \*Higher conductivity in doped ethylenedioxythiophene (EDOT) dimers with chalcogen-substituted end groups: K. Onozuka, T. Fujino, T. Miyamoto, T. Yamakawa, H. Okamoto, H. Akiba, O. Yamamuro, E. Kayahara, S. Yamago, H. Oike and H. Mori, *J. Mater. Chem. C* **12**, 13956 (2024).

## 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; inelastic neutron scattering study on Skyrmion host compound GaV<sub>4</sub>Se<sub>8</sub>, chiral split magnon in altermagnetic MnTe, field control of quasiparticle decay in a quantum antiferromagnet, spin dynamics in equilateral triangular spin tube material CsCrF<sub>4</sub> and so on. We also developed a new inelastic neutron spectrometer HODACA.

1. A New Inelastic Neutron Spectrometer HODACA: H. Kikuchi, S. Asai, T. J. Sato, T. Nakajima, L. Harriger, I. Zaliznyak and T. Masuda, *J. Phys. Soc. Jpn.* **93**, 091004(1-11) (2024).
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4. †\*Elastic and inelastic neutron scattering experiments under high pressure in the frustrated antiferromagnet CuFeO<sub>2</sub>: N. Terada, D. D. Khalyavin, P. Manuel, S. Asai, T. Masuda, H. Saito, T. Nakajima and T. Osakabe, *Phys. Rev. B* **110**, 024406 (2024).
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7. Chiral Split Magnon in Altermagnetic MnTe: Z. Liu, M. Ozeki, S. Asai, S. Itoh and T. Masuda, *Phys. Rev. Lett.* **133**, 156702(1-6) (2024).
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## Nakajima group

Nakajima group is studying magnetic materials with cross-correlated phenomena associated with the symmetry of the magnetic structures by means of neutron and X-ray scattering techniques. We are responsible for a polarized-neutron triple-axis neutron spectrometer PONTA in the research reactor JRR-3 in Tokai, and have been supporting the users of the ISSP-NSL joint-use program. One of the research highlights at PONTA in the fiscal year of 2024 is the discovery of a non-coplanar helimagnetic order in the van der Waals compound  $\text{DyTe}_3$ . Prof. Hirschberger's group in the university of Tokyo grew a single crystal of this compound, and performed neutron diffraction measurements at PONTA. They revealed that commensurate and incommensurate magnetic peaks emerge below the antiferromagnetic transition temperature of  $T_N = 3.85$  K, which was determined by magnetic susceptibility and heat capacity measurements. By utilizing the polarized neutron scattering technique, they successfully elucidated that the magnetic structure of this compound is an alternating transverse conical magnetic structure. The complex helimagnetic ordering on cleavable van der Waals layers would be potentially applicable for spintronics devices. Nakajima group is also working on developing new neutron scattering techniques in extreme conditions. In this fiscal year, we have published a paper reporting neutron time-of-flight diffraction measurements in long pulsed-magnetic fields in collaboration with Prof. Kohama's group in IMGSL of ISSP. By combining the high-intensity pulsed neutron beam in J-PARC and long pulsed magnetic field developed by Prof. Kohama, we successfully observed diffraction patterns corresponding to field induced magnetic phases in a triangular lattice antiferromagnet  $\text{CuFe}_{1-x}\text{Ga}_x\text{O}_2$ . We are planning to introduce spin-polarization analyzer for scattered neutrons, which enables us to determine the symmetry of the magnetic structure from a limited number of magnetic reflections, in the future.

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## Mayumi group

Contrast variation small-angle neutron scattering (CV-SANS) is a powerful tool to evaluate the structure of multi-component systems by decomposing scattering intensities  $I(Q)$  measured with different scattering contrasts into partial scattering functions  $S(Q)$  of self- and cross-correlations between components. The measured  $I(Q)$  contains a measurement error,  $\Delta I(Q)$ , and  $\Delta I(Q)$  results in an uncertainty of partial scattering functions,  $\Delta S(Q)$ . However, the error propagation from  $\Delta I(Q)$  to  $\Delta S(Q)$  has not been quantitatively clarified. We have established deterministic and statistical approaches to determine  $\Delta S(Q)$  from  $\Delta I(Q)$ . We have applied the two methods to (i) computational data of a core-shell sphere and experimental CV-SANS data of (ii) clay/polyethylene glycol (PEG) aqueous solutions and (iii) polyrotaxane solutions, and have successfully estimated the errors of  $S(Q)$ . The quantitative error estimation of  $S(Q)$  offers us a strategy to optimize the combination of scattering contrasts to minimize error propagation.

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## Kofu group

Our laboratory started in January 2025. We study the dynamics of atoms, molecules, and spins in various materials using neutron scattering techniques to discover novel phenomena and universality inherent in a wide range of materials. In this financial year, we performed inelastic/quasielastic scattering measurements of Ising spin glass (Fe,Mn)TiO<sub>3</sub>, martyite, and amorphous metal hydride PdSiH using AMATERAS at J-PARC and AGNES at JRR-3. We also supported user experiments on liquids, hydrates, and polymer systems using AGNES and contributed in part to the joint-use operation of AMATERAS.

## International MegaGauss Science Laboratory

### Kindo group

We have found the process of fabricating the Cu-Ag wire for a stable 85 T shot. Every coil wound by the new wire can generate the magnetic field exceeding 85 T without failure in this year.

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## Tokunaga group

Magnetization measurements in pulsed magnetic fields up to 66 T in a honeycomb lattice antiferromagnet  $\text{Fe}_2\text{Mo}_3\text{O}_8$  with strong Ising magnetic anisotropy revealed a six-step magnetization plateau. The results of electric polarization measurements also showed plateaus corresponding to the magnetization process. We successfully reproduce these plateaus in a model that includes the interaction between the second-nearest neighbor spins.

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## Y. Matsuda group

We have studied the magnetic field-induced phase transitions in several intriguing magnetic materials, LaCoO<sub>3</sub>, Ho<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>, Pr<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub>, and a layered, spin- 1/2 organic-inorganic copper sulfate. Also, we have investigated the strong anisotropic magnetization process in a potential permanent magnet, SmCo<sub>4</sub>B. In addition to the compounds mentioned above, several materials, including a ferroelectric material, transition metal intermetallic compounds, and organic solids, have been studied by several techniques such as the dielectric constant measurement, electric impedance measurement, magnetostriction measurement, and streak camera spectroscopy. The aim of the recent research of our group is to explore the unique non-perturbative magnetic field effect (NPME) in ultrahigh magnetic fields exceeding 100 T. One of the typical NPMEs is the field-induced crystal structural change, which should be interpreted as the modification of the chemical bond in a solid in some sense. The strong spin-lattice coupling is the key physical parameter and can lead to the discovery of novel crystals appear only in an ultrahigh magnetic field.

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## Kohama group

We have investigated high-field properties on several compounds. In itinerant systems, such as CeCoSi and YbB<sub>12</sub>, the field-induced anomalies have been investigated by calorimetry and magnetic transport experiments using non-destructive pulsed magnetic fields. Here we also collaborated with the Grenoble high-field laboratory and IMR. In magnetic materials, we have investigated the spin-lattice coupling in destructive pulsed fields. We have also developed the J<sub>c</sub> measurement technique in pulsed fields for the application to the applied superconductivity.

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## Miyata group

We have worked on magneto-optical experiments under pulsed magnetic fields to search for exotic magneto-optical phenomena in antiferromagnets (especially, van der Waals antiferromagnets). The magnetoelectric material  $\text{LiNiPO}_4$  has complex magnetic exchange interactions, leading to a sequence of magnetic phase transitions in high magnetic fields. Our pulsed field experiments revealed that  $\text{LiNiPO}_4$  exhibits complex linear dichroism (LD) and directional dichroism (DD), arising from low magnetic symmetries induced by high magnetic fields. The vdW antiferromagnet  $\text{NiI}_2$  is the first known candidate to show multiferroicity even at the atomic layer scale. It also shows magnetic excitons that are strongly coupled to its magnetic structure. Our experiments demonstrated that the magnetic exciton shows a shoulder-like structure between 20-30 T and undergoes a significant shift above 30 T due to magnetic phase transitions.

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# Center of Computational Materials Science

## Misawa group

We have developed numerical methods and software packages for strongly correlated electron systems. We have updated HΦ (software for exact diagonalization), many-variable variational Monte Carlo method (mVMC), and released H-wave (software for Hartree-Fock calculations and random phase approximations). Using these software packages, we have performed *ab initio* calculations for molecular solids, and a variational Monte Carlo study for the Kondo lattice model on a triangular lattice.

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## Inui group

We advanced an automatic-differentiation-driven inverse-design platform for quantum-material functionalities. The major achievements in 2024 are (1) optimizing disorder landscapes in mesoscopic conductors to precisely reproduce target magnetotransport responses, and (2) designing spin-exchange Hamiltonians that maximize many-body entanglement, naturally yielding quantum-spin-liquid ground states. These results showcase computation-guided inverse design as a versatile route to engineer electronic and magnetic properties from the nanoscale upward.

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# Laser and Synchrotron Research Center

## Kobayashi group

Laser Development and cyber physical system

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## Harada group

In 2024, we utilized soft X-ray absorption (XAS) and resonant emission spectroscopy (RXES) to investigate advanced materials for energy storage and the behavior of water in confined environments. We elucidated the charge compensation mechanisms in layered oxyfluorides and oxyfluorosulfides for fluoride-ion batteries, revealing anion redox processes that enable high capacities of 200-340 mAh/g. The XES studies on water structure yielded insights into hydrogen bonding configurations in various systems, including polymer interfaces, nanochannels, and zwitterionic block copolymers. We correlated these molecular-level water structures to macroscopic properties such as biocompatibility and material functionality. The oxygen K-edge XES measurements on metal-organic frameworks revealed the electronic perturbations driving structural breathing transitions through carboxylate oxygen lone pair orbital reconfigurations. To enhance our analytical capabilities, we implemented a sophisticated rotation mechanism to the X-ray emission spectrometer that enables flexible scattering angle adjustments between 45-135°. This advancement streamlines angle-resolved XES measurements and expands its versatility to include diffraction experiments.

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## I. Matsuda group

The new synchrotron radiation facility, NanoTerasu, was launched at Sendai in Miyagi-prefecture and we started the user operation with our end-stations at the soft X-ray beamline BL08U. At the station of ambient-pressure X-ray spectroscopy, we have made experiments with users on gas/solid interfaces of various materials, such as model catalysts. We have also upgraded the instrument and succeeded in measuring soft X-ray photoelectron spectra at the real ambient pressure condition (1 bar). The achievement is for the first time in human history and it has opened the real operando experiments on the real functional materials. At the station of X-ray spectromicroscopy, two-dimensional scan of X-ray absorption spectroscopy can be performed with automatic controls. The system has continuously been developed as the autonomous robot system with process-informatics.

Our group has conducted synthesis of the boron materials by the film growth and the subsequent chemical exfoliations. On copper crystal surface, we have discovered one-dimensional (1-D) structure with quasi-periodicity. We have also succeeded in growing millimeter-sized crystals of 3-D metal boride and 2-D hydrogen boride. These novel materials are expected to provide various functionalities that will be useful in our society.

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## Itatani group

The enhancement of harmonic generation in thin water jets under intense mid-infrared excitation is found to be due to the creation of novel high temperature and high pressure state of water caused by resonant vibrational excitation and hydrogen bond perturbation. We have also experimentally clarified the superluminal propagation associated with strong resonant absorption in the 2.9- $\mu\text{m}$  band. These experiments using a thin flat liquid jet demonstrate a new platform for attosecond experiments of condensed matter using intense laser fields. We have also started the development of a Cr:ZnSe solid-state laser amplifier to realize a high-intensity infrared source at 2  $\mu\text{m}$ . We also started the development of a femtosecond VUV source with a repetition rate of 100 kHz at a photon energy of 11 eV for ultrafast angle-resolved photoemission spectroscopy.

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## Kondo group

We uncovered novel electronic phenomena in correlated and topological materials. Using ARPES, we demonstrated that Fermi surface nesting drives skyrmion formation in centrosymmetric  $\text{Gd}_2\text{PdSi}_3$  and discovered anomalous Fermi pockets on the Hund's metal surface of  $\text{Sr}_2\text{RuO}_4$  due to enhanced spin-orbit coupling. We also visualized symmetry-protected spin-polarized states in bismuth and identified gap features in Dirac semimetals. These studies deepen our understanding of nontrivial topological states, magnetic interactions, and quantum coherence, contributing broadly to the design of future spintronic and quantum materials.

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## Matsunaga group

We have studied light-matter interactions and light-induced nonequilibrium phenomena in solids by utilizing terahertz (THz) pulse. By using polarization-resolved THz spectroscopy and a semiconductor GaAs, we have reported the first observation of spin Hall conductivity spectrum of electrons. The frequency dependence of spin Hall conductivity exhibits an excellent quantitative agreement with theory, demonstrating a crossover in the dominant origin from impurity scattering in the dc regime to the intrinsic Berry-curvature mechanism in the terahertz regime. Our spectroscopic technique opens a new pathway to analyze anomalous transports. In addition, we successfully generated phase-stable counterrotating bicircular light pulses in the 14–39 THz frequency range. Use of the spatial light modulator enabled programmable control over the shape, orientation, rotational symmetry, and helicity of the bicircular light field trajectory. This advancement provides a novel pathway for the programmable manipulation of light fields.

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## 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 photoexcited non-equilibrium states by a time-resolved ARPES apparatus using EUV and SX lasers. In the academic year 2024, we investigated the superconducting gap structure of the iron-based superconductor  $BaNaFeAs$  with a reentrant  $C_4$  phase by high-resolution laser ARPES. In addition, we successfully observed a photoinduced modulation of the van Hove singularity in the kagome superconductor  $CsVSb$  by HHG laser time-resolved ARPES.

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## Kimura group

In fiscal year 2024, we worked on the development and application of soft X-ray microscopy systems using SPring-8 BL07LSU and SACLA BL1. We attempted to measure mammalian cells using soft X-ray ptychography with a total reflection Wolter mirror, and performed live cell imaging with a single femtosecond X-ray free-electron laser pulse and intracellular chemical state mapping combined with soft X-ray spectro-microscopy.

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† Joint research with outside partners.

\* Joint research between groups within ISSP.