Publications (2023.1 - 2024.4)

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 2023 are to develop the metallic oligomer conductors that models doped PEDOT [poly(3,4-ethylene-dioxythiophene)] family and (2) to discover the high conductive mixed-stack complexes via orbital hybridization of donor and acceptor.

1. †*Ambipolar Nickel Dithiolene Complex Semiconductors: From One- to Two-Dimensional Electronic Structures Based upon Alkoxy Chain Lengths: M. Ito, T. Fujino, L. Zhang, S. Yokomori, T. Higashino, R. Makiura, K. J. Takeno, T. Ozaki and H. Mori, J. Am. Chem. Soc. **145**, 2127-2134 (2023).

2. †*Metallic State of a Mixed-Sequence Oligomer Salt That Models Doped PEDOT Family: K. Onozuka, T. Fujino, R. Kameyama, S. Dekura, K. Yoshimi, T. Nakamura, T. Miyamoto, T. Yamakawa, H. Okamoto, H. Sato, T. Ozaki and H. Mori, J. Am. Chem. Soc. **145**, 15152-15161 (2023).

3. †Neutral Radical Molecular Conductors Based on a Gold Dimethoxybenzenedithiolene Complex with and without Crystal Solvent: S. Yokomori, S. Dekura, A. Ueda, T. Higashino and H. Mori, Chem. Lett. **52**, 25 (2023).

4. †*Precise Control of the Molecular Arrangement of Organic Semiconductors for High Charge Carrier Mobility: R. Akai, K. Oka, S. Dekura, K. Yoshimi, H. Mori, R. Nishikubo, A. Saeki and N. Tohnai, J. Phys. Chem. Lett. **14**, 3461 (2023).

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).

6. 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).

7. 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

The electronic state under magnetic fields in the α-type organic Dirac fermion systems, α-$(ET)_2I_3$ and α-$(BETS)_2I_3$, was studied to clarify the spatial order in the quantum Hall state. The four-band tight-binding model with Peierls phase factors was employed, and the generated Hofstadter butterfly and its Chern numbers confirmed the validity of the Dirac fermion picture in these materials. The four-component envelope function of the $N = 0$ Landau level with valley degeneracy was investigated. It was found that the two degenerate valley states have different weights on A and A' molecules connected by inversion. This valley-site correspondence is also recognized for the $N = 0$ spin-split Landau levels under the Zeeman effect and the spin–orbit interaction. The spontaneous valley symmetry breaking in the $N = 0$ Landau levels due to the exchange interaction results in the $\nu = \pm 1$ quantum Hall states accompanied by the spatial modulation of charge and spin densities at A and A' sites in a unit cell.

1. Magnetic-field periodic quantum Sondheimer oscillations in thin-film graphite: T. Taen, A. Kiswandhi and T. Osada, Phys. Rev. B **108**, 235411(1-9) (2023).

2. Quantized thermoelectric Hall plateau in the quantum limit of graphite as a nodal-line semimetal: A. Kiswandhi, T. Ochi, T. Taen, M. Sato, K. Uchida and T. Osada, Phys. Rev. B **107**, 195106(1-5) (2023).

3. Broken-Symmetry Quantum Hall State in an Organic Dirac Fermion System: T. Osada, JPSJ News Comments **20**, 06 (2023).

4. Hofstadter Butterfly and Broken-Symmetry Quantum Hall States in α -Type Organic Dirac Fermion Systems: T. Osada,

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* Joint research among groups within ISSP.

J. Phys. Soc. Jpn. **93**, 034711(1-6) (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 thermal conductivity and magnetization measurements of a quantum spin ice candidate $Ce_2Hf_2O_7$ (2) spontaneous thermal Hall measurements of candidate materials of chiral superconductivity, and (3) NMR measurements of $Cd_2Re_2O_7$.

1. †*Modulation vector of the Fulde-Ferrell-Larkin-Ovchinnikov state in CeCoIn5 revealed by high-resolution magnetostriction measurements: S. Kittaka, Y. Kono, K. Tsunashima, D. Kimoto, M. Yokoyama, Y. Shimizu, T. Sakakibara, M. Yamashita and K. Machida, Phys. Rev. B **107**, L220505 (2023).

2. Magnon thermal Hall effect via emergent 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).

Ideue group

We have studied novel transport and optical properties of two-dimensional materials. We have successfully observed circular bulk photovoltaic effect at heterointerfaces of two-dimensional materials with different symmetries, which reflect the geometric nature of the electronic state. We have also shown that the anisotropy of transport and optical properties can be controlled in such symmetry-engineered van der Waals interfaces. Furthermore, we have reported a giant modulation of second harmonic generation in layered multiferroic $CuCrP_2S_6$ and its unique thickness dependence.

1. Valley-dimensionality locking of superconductivity in cubic phosphides: L. Ao, J. Huang, F. Qin, Z. Li, T. Ideue, K. Akhtari, P. Chen, X. Bi, C. Qiu, D. Huang, L. Chen, R. V. Belosludov, H. Gou, W. Ren, T. Nojima, Y. Iwasa, M. S. Bahramy and H. Yuan, Sci. Adv. **9**, eadf6758 (2023).

2. An anisotropic van der Waals dielectric for symmetry engineering in functionalized heterointerfaces: Z. Li, J. Huang, L. Zhou, Z. Xu, F. Qin, P. Chen, X. Sun, G. Liu, C. Sui, C. Qiu, Y. Lu, H. Gou, X. Xi, T. Ideue, P. Tang, Y. Iwasa and H. Yuan, Nat Commun **14**, 5568 (2023).

3. Low-temperature phase transition in polar semimetal Td−MoTe2 probed by nonreciprocal transport: Y. M. Itahashi, Y. Nohara, T. Ideue, T. Akiba, H. Takahashi, S. Ishiwata and Y. Iwasa, Phys. Rev. Research **5**, L022022 (2023).

4. Berry curvature dipole generation and helicity-to-spin conversion at symmetry-mismatched heterointerfaces: S. Duan, F. Qin, P. Chen, X. Yang, C. Qiu, J. Huang, G. Liu, Z. Li, X. Bi, F. Meng, X. Xi, J. Yao, T. Ideue, B. Lian, Y. Iwasa and H. Yuan, Nat. Nanotechnol. **18**, 867 (2023).

5. Giant bulk piezophotovoltaic effect in 3R-MoS2: Y. Dong, M.-M. Yang, M. Yoshii, S. Matsuoka, S. Kitamura, T. Hasegawa, N. Ogawa, T. Morimoto, T. Ideue and Y. Iwasa, Nat. Nanotechnol. **18**, 36-41 (2023).

6. Continuous manipulation of magnetic anisotropy in a van der Waals ferromagnet via electrical gating: M. Tang, J. Huang, F. Qin, K. Zhai, T. Ideue, Z. Li, F. Meng, A. Nie, L. Wu, X. Bi, C. Zhang, L. Zhou, P. Chen, C. Qiu, P. Tang, H. Zhang, X. Wan, L. Wang, Z. Liu, Y. Tian, Y. Iwasa and H. Yuan, Nat. Electron. **6**, 28-36 (2023).

7. Giant Modulation of the Second Harmonic Generation by Magnetoelectricity in Two-Dimensional Multiferroic CuCrP2S6: 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

We have been exploring new properties and functions related to topological magnetic structures, and novel electronic phases in strongly correlated electron systems. This year, we investigated the spontaneous topological Hall effect induced by non-coplanar antiferromagnetic order in intercalated van der Waals compounds. We also revealed the contribution of lattice degree of freedom to the rhombic and square lattice states of skyrmions in $EuAl_4$.

1. *Nonreciprocal Phonon Propagation in a Metallic Chiral Magnet: T. Nomura, X. -X. Zhang, R. Takagi, K. Karube, A. Kikkawa, Y. Taguchi, Y. Tokura, S. Zherlitsyn, Y. Kohama and S. Seki, Phys. Rev. Lett. **130**, 176301(1-6) (2023).

2. *Spontaneous topological Hall effect induced by non-coplanar antiferromagnetic order in intercalated van der Waals materials: H. Takagi, R. Takagi, S. Minami, T. Nomoto, K. Ohishi, M. -T. Suzuki, Y. Yanagi, M. Hirayama, N. D.

† Joint research with outside partners.

Khanh, K. Karube, H. Saito, D. Hashizume, R. Kiyanagi, Y. Tokura, R. Arita, T. Nakajima and S. Seki, Nat. Phys. **19**, 961-968 (2023).

3. SP-STM study of the multi-Q phases in GdRu2Si2: 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).

Division of Condensed Matter Theory

Tsunetsugu group

We have studied various quadrupole orders on face center cubic lattice. This system has a few important points characteristic to quadrupole degrees of freedom. One is the presence of anisotropic interactions reflecting tensorial nature of the order parameter. Another is the third-order anisotropy, which exists only for degrees of freedom with even parity concerning time reversal symmetry. We have found various types of antiferro orders and discussed their stability based on phonemenological Landau theory. We have also studied a quadrupole impurity embedded in a host metal. Using the Wilson-type numerical renormalization technique, we have examined the related two-channel Kondo problem with taking account of the third-order local anisotropy taken into account. We have found two fixed points; one is the conventional local Fermi liquid and the other is the non-Fermi liquid, which is stable in a finite region of the parameter space. We have performed detailed analysis about the Kondo temperature in the local Fermi liquid phase. The Kondo temperature has a scaling behavior that differs from the conventional form, and the determined scaling function demonstrates the relevance of multiple coupling constants in the renormalization group equation.

1. †Theory of Energy Dispersion of Chiral Phonons: H. Tsunetsugu and H. Kusunose, J. Phys. Soc. Jpn. **92**, 023601 (2023).

2. Quadrupole partial orders and triple-q states on the face-centered cubic lattice: K. Hattori, T. Ishitobi and H. Tsunetsugu, Phys. Rev. B **107**, 205126 (2023).

3. All Local Conserved Quantities of the One-Dimensional Hubbard Model: K. Fukai, Phys. Rev. Lett. **131**, 256704 (2023).

4. Matrix product operator representations for the local conserved quantities of the Heisenberg chain: K. Yamada and K. Fukai, SciPost Phys. Core **6**, 069 (2023).

5. 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).

6. On correlation functions in models related to the Temperley-Lieb algebra: K. Fukai, R. Kleinemühl, 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 studied (1) spin pumping into two-dimensional electron gas and current induced by it, (2) ultrafast rotation of nanoparticles driven by ferromagnetic resonance and its quantum fluctuation, (3) spin pumping into twisted bilayer graphene and carbon nanotubes, (4) minimum ac injection into one-dimensional electron systems. We also published collaborated work with experimental group in ISSP about ac spin Hall effect.

1. Effect of vertex corrections on the enhancement of Gilbert damping in spin pumping into a two-dimensional electron gas: M. Yama, M. Matsuo and T. Kato, Phys. Rev. B **107**, 174414(1-15) (2023).

2. Gyromagnetic bifurcation in a levitated ferromagnetic particle: T. Sato, T. Kato, D. Oue and M. Matsuo, Phys. Rev. B **107**, L180406(1-6) (2023).

3. Minimal alternating current injection into carbon nanotubes: K. Fukuzawa, T. Kato, T. Jonckheere, J. Rech and T. Martin, Phys. Rev. B **108**, 125307(1-12) (2023).

4. Quantum fluctuation in rotation velocity of a levitated magnetic particle: T. Sato, D. Oue, M. Matsuo and T. Kato, Phys. Rev. B **108**, 094428(1-10) (2023).

5. *Shear-strain controlled high-harmonic generation in graphene: T. Tamaya, H. Akiyama and T. Kato, Phys. Rev. B **107**, L081405 (2023).

* Joint research among groups within ISSP.

6. Spin Hall magnetoresistance in quasi-two-dimensional antiferromagnetic-insulator/metal bilayer systems: T. Ishikawa, M. Matsuo and T. Kato, Phys. Rev. B **107**, 054426 (2023).

7. Spin Hall magnetoresistive detection of easy-plane magnetic order in the van der Waals antiferromagnet $NiPS_3$: K. Sugi, T. Ishikawa, M. Kimata, Y. Shiota, T. Ono, T. Kato and T. Moriyama, Phys. Rev. B **108**, 064434 (2023).

8. Spin pumping into carbon nanotubes: K. Fukuzawa, T. Kato, M. Matsuo, T. Jonckheere, J. Rech and T. Martin, Phys. Rev. B **108**, 134429(1-9) (2023).

9. Theory of inverse Rashba-Edelstein effect induced by spin pumping into a two-dimensional electron gas: M. Yama, M. Matsuo and T. Kato, Phys. Rev. B **108**, 144430 (2023).

10. Twisted bilayer graphene reveals its flat bands under spin pumping: S. Haddad, T. Kato, J. Zhu and L. Mandhour, Phys. Rev. B **108**, L121101 (2023).

11. Nonequilibrium noise as a probe of pair-tunneling transport in the BCS–BEC crossover: H. Tajima, D. Oue, M. Matsuo, T. Kato and D. Abbott, PNAS Nexus **2**, pgad045 (2023).

12. *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 (2024).

13. †*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).

14. †*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).

15. 磁気的界面を通じて超伝導対称性を視る—強磁性共鳴変調を用いたスペクトロスコピー—: 大湊 友也 , 山影 相 , 加藤 岳生 , 松尾 衛 , 固体物理 **58**, 433-440 (2023).

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. *Dynamical quantum phase transitions in Sachdev-Ye-Kitaev Lindbladians: K. Kawabata, A. Kulkarni, J. Li, T. Numasawa and S. Ryu, Phys. Rev. B **108**, 075110 (2023).

2. Non-Hermitian boost deformation: T. Guo, K. Kawabata, R. Nakai and S. Ryu, Phys. Rev. B **108**, 075108 (2023).

3. Symmetry classification of typical quantum entanglement: Y. Liu, J. Kudler-Flam and K. Kawabata, Phys. Rev. B **108**, 085109 (2023).

4. Anisotropic Topological Anderson Transitions in Chiral Symmetry Classes: Z. Xiao, K. Kawabata, X. Luo, T. Ohtsuki and R. Shindou, Phys. Rev. Lett. **131**, 056301 (2023).

5. Hermitian Bulk – Non-Hermitian Boundary Correspondence: F. Schindler, K. Gu, B. Lian and K. Kawabata, PRX Quantum **4**, 030315 (2023).

6. Singular-Value Statistics of Non-Hermitian Random Matrices and Open Quantum Systems: K. Kawabata, Z. Xiao, T. Ohtsuki and R. Shindou, PRX Quantum **4**, 040312 (2023).

7. *Symmetry of Open Quantum Systems: Classification of Dissipative Quantum Chaos: K. Kawabata, A. Kulkarni, J. Li, T. Numasawa and S. Ryu, PRX Quantum **4**, 030328 (2023).

8. 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).

9. Lieb-Schultz-Mattis Theorem in Open Quantum Systems: K. Kawabata, R. Sohal and S. Ryu, Phys. Rev. Lett. **132**, 070402 (2024).

† Joint research with outside partners.

Division of Nanoscale Science

Otani group

Our research in 2023 spans diverse investigations on spin-mediated quasiparticles' interconversions and their intricate interactions. One study dissects the efficiency of orbital torque within ferromagnet/Cu/oxide heterostructures, emphasizing the pivotal role of oxide layers in this process. Another delves into the domain evolution and structure of Mn_3Ge, an intriguing noncollinear Weyl antiferromagnet, spotlighting the presence and behavior of magnetic octupole domains. Acoustic waves are scrutinized for their impact on magnon dynamics in layered antiferromagnets, revealing acoustically induced magnon-phonon coupling phenomena. Furthermore, we explored the manipulation of magnon transport through valley-selective phonon-magnon scattering in magnetoelastic superlattices, offering a pathway for controlling magnetic information transfer. The investigation extends to nonlinear acoustic spin pumping driven by temperature-dependent surface acoustic wave frequency shifts, elucidating nuanced spin-phonon interactions. Additional studies employ innovative techniques like tip-induced temperature gradients in atomic force microscopy to map magneto-thermoelectric effects, providing insights into magnetic domain structure consisting of antiferromagnetic octupoles. These findings collectively advance our comprehension of noncollinear antiferromagnetic materials and their multifaceted behaviors, contributing to the evolution of spintronics and related fields.

1. Nonlinear Acoustic Spin Pumping Caused by Temperature-Dependent Frequency Shifts of Surface Acoustic Waves: Y. Hwang, J. Puebla, K. Kondou, C. S. Muñoz and Y. Otani, J. Phys. Soc. Jpn. **92**, 094702 (2023).
2. Acoustically Driven Magnon-Phonon Coupling in a Layered Antiferromagnet: T. P. Lyons, J. Puebla, K. Yamamoto, R. S. Deacon, Y. Hwang, K. Ishibashi, S. Maekawa and Y. Otani, Phys. Rev. Lett. **131**, 196701 (2023).
3. Valley-Selective Phonon-Magnon Scattering in Magnetoelastic Superlattices: L. Liao, J. Puebla, K. Yamamoto, J. Kim, S. Maekawa, Y. Hwang, Y. Ba and Y. Otani, Phys. Rev. Lett. **131**, 176701 (2023).
4. [*]High-resolution magnetic imaging by mapping the locally induced anomalous Nernst effect using atomic force microscopy: N. Budai, H. Isshiki, R. Uesugi, Z. Zhu, T. Higo, S. Nakatsuji and Y. Otani, Appl. Phys. Lett. **122**, 102401 (2023).
5. Mid-infrared optical properties of non-magnetic-metal/CoFeB/MgO heterostructures: J. M. Flores-Camacho, B. Rana, R. E. Balderas-Navarro, A. Lastras-Martínez, Y. Otani and J. Puebla, J. Phys. D: Appl. Phys. **56**, 315301 (2023).
6. [*]Temperature-induced anomalous magnetotransport in the Weyl semimetal Mn_3Ge: M. Wu, K. Kondou, T. Chen, S. Nakatsuji and Y. Otani, AIP Advances **13**, 045102 (2023).
7. Emergence of spin–charge conversion functionalities due to spatial and time-reversal asymmetries and chiral symmetry: K. Kondou and Y. Otani, Front. Phys. **11**, 1140286 (2023).
8. [†*]Oxide layer dependent orbital torque efficiency in ferromagnet/Cu/oxide heterostructures: J. Kim, J. Uzuhashi, M. Horio, T. Senoo, D. Go, D. Jo, T. Sumi, T. Wada, I. Matsuda, T. Ohkubo, S. Mitani, H.-W. Lee and Y. Otani, Phys. Rev. Materials **7**, L111401 (2023).
9. Magnetic octupole domain evolution and domain-wall structure in the noncollinear Weyl antiferromagnet Mn3Ge: M. Wu, K. Kondou, Y. Nakatani, T. Chen, H. Isshiki, T. Higo, S. Nakatsuji and Y. Otani, AIP Publishing **11**, 081115 (2023).

Hasegawa group

We implemented the potentiometry function, which enabled us to observe the surface electrochemical potential profile and spatial distribution of resistance at sub-nanometer spatial resolution, using low-temperature scanning tunneling microscopy (STM). Using this setup, we can investigate potential profiles in a more stable manner under various temperatures and magnetic fields (up to 7 T). The temperature profile of the surface can also be investigated by detecting the Seebeck thermoelectric power. Using this system, we investigated the striped incommensurate (SIC) phase of a Pb monolayer formed on a non-doped Si(111) substrate. The structure is known to be metallic and exhibit superconductivity at low temperatures. Our previous study observing vortices pinned at steps demonstrated that the resistivity across a single height step is small. The small resistivity was proved directly through the observation of potential differences across single-height steps. We also performed magnetic-field-dependent potential profile measurements and successfully probed the Hall voltage locally in the nanoscale area, providing information on the charge carrier and density of the two-dimensional monolayer metallic states. We plan to investigate quantum nonlocal potential phenomena, as well as classical local phenomena in real space.

1. Squeezed Abrikosov-Josephson Vortex in Atomic-Layer Pb Superconductors Formed on Vicinal Si(111) Substrates: Y. Sato, M. Haze, R. Nemoto, W. Qian, S. Yoshizawa, T. Uchihashi and Y. Hasegawa, Phys. Rev. Lett. **130**, 106002(1-6) (2023).
2. [†*]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.

[*] Joint research among groups within ISSP.

Kondo and I. Matsuda, Nano Lett. **24**, 1160 (2024).

Lippmaa group

We are developing a new autonomous synthesis method for thin films. Structural information on a thin film is obtained during growth by monitoring RHEED patterns. The diffraction images are semantically segmented using a neural network to locate various diffraction features, such as surface streaks, surface diffraction spots, bulk diffraction spots, the direct electron beam location, the Kikuchi lines, etc. The extracted data is used for periodicity analysis and lattice parameter data clustering, which produces a phase composition estimate of a growing crystal. This information is used in a Gaussian process optimization to predict the best process parameters for the film growth to obtain the desired crystalline phase.

1. *Semiconducting Electronic Structure of the Ferromagnetic Spinel $HgCr_2Se_4$ Revealed by Soft-X-Ray Angle-Resolved Photoemission Spectroscopy: H. Tanaka, A. V. Telegin, Y. P. Sukhorukov, V. A. Golyashov, O. E. Tereshchenko, A. N. Lavrov, T. Matsuda, R. Matsunaga, R. Akashi, M. Lippmaa, Y. Arai, S. Ideta, K. Tanaka, T. Kondo and K. Kuroda, Phys. Rev. Lett. **130**, 186402(1-6) (2023).

2. *Fabrication of single-crystalline $YFeO_3$ films with large antiferromagnetic domains: C. Wang, M. Lippmaa and S. Nakatsuji, J. Appl. Phys. **135**, 113901(1-8) (2024).

3. †The use of He buffer gas for moderating the plume kinetic energy during Nd:YAG-PLD growth of $Eu_xY_{2-x}O_3$ 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).

5. 機械学習による意思決定とデータ解釈：物質合成パラメータの最適化と in situ 測定結果の自動解析 : 大久保 勇男 and M. Lippmaa,「ケモインフォマティクスにおけるデータ収集の最適化と解析手法」, 5, (株式会社技術情報協会 , Tokyo, 2023), 359-366.

Hashisaka group

Our group was newly inaugurated at ISSP in April 2023. We are working on setting up equipment for electrical transport measurements at cryogenic temperatures, and the experimental environment is being prepared. While working on these startups, we also worked on the edge transport mechanism at a fractional-integer quantum Hall junction and the evaluation of superconducting nonreciprocal transport phenomena in few-layer Td-MoTe2. We also studied the single-electron coherence in interacting copropagating integer quantum Hall edge channels, where an electron experiences fractionalization due to the Tomonaga-Luttinger liquid nature.

1. Coherent-Incoherent Crossover of Charge and Neutral Mode Transport as Evidence for the Disorder-Dominated Fractional Edge Phase: M. Hashisaka, T. Ito, T. Akiho, S. Sasaki, N. Kumada, N. Shibata and K. Muraki, Phys. Rev. X **13**, 031024 (2023).

2. Gate-tunable giant superconducting nonreciprocal transport in few-layer Td-MoTe2: 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).

Yoshinobu group

We conducted several research projects in the fiscal year 2023: (1) The hydrogenation of formate species on the H-Cu(997) surface was studied by HREELS and TPD. Desorption of formaldehyde was observed by TPD, and a possible intermediate species was investigated. (2) The adsorption and decomposition of methanol on the Cu(977) and Pd-Cu(977) surfaces were studied by TPD, IRAS and SR-XPS. (3) The reactive desorption of CO + O -> CO_2 on Pt(111) was studied using ab-initio molecular dynamics (AIMD) with van der Waals DFT functionals. The desorption dynamics of CO_2 including kinetic energy, angular distribution and vibrational excitation were analyzed. (4) The chemical states and reactions on the basal plane and the edge plane of MoS_2 were studied in vacuum and under the exposure to water or CO_2 by SR-XPS. (5) Gapless detection of broadband terahertz pulses using a metal surface was newly developed. (6) SFG spectroscopy was developed using broadband terahertz and visible ultra-short pulse laser.

1. *Disentangling the Competing Mechanisms of Light-Induced Anomalous Hall Conductivity in Three-Dimensional Dirac Semimetal: Y. Murotani, N. Kanda, T. Fujimoto, T. Matsuda, M. Goyal, J. Yoshinobu, Y. Kobayashi, T. Oka, S. Stemmer and R. Matsunaga, Phys. Rev. Lett. **131**, 096901 (2023).

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Functional Materials Group

Akiyama group

In 2023, we accomplished ultra-fast gain-switching experiment in 30GHz-modulation-bandwidth 1270nm DFB-type single-mode laser diodes (LDs) with and without chirp compensation, and analyzed generated 5.3 ps short pulses near the Fourier transform limit via rate equations and other laser theory framework. We developed our original 10 ps LD-seed-pulse prototype modules with improvements in packaging and software. We extended our high-efficiency-solar-cell study to efficient power conversion of laser light, and achieved high conversion efficiency of about 50%. Collaboration work and papers with Hiyama-team in Gunma University were accomplished on quantitative spectroscopy on bioluminescence quantum yield of new luciferin analogs.

1. *Shear-strain controlled high-harmonic generation in graphene: T. Tamaya, H. Akiyama and T. Kato, Phys. Rev. B **107**, L081405 (2023).

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* Joint research among groups within ISSP.

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Sugino group

This year, this group performed first-principles calculations of the structure of water-Pt(111) interface, oxygen reduction reaction on a defective ZrO_2 surface, quantum mechanical hydrogen diffusion on noble metal surfaces, magnetic structure of a supercondunting cuprate material $Sr_{1-x}La_xCuO_2$. In addition, a model Hamiltonian was used study the nonadiabatic quantum dynamics of an electrochemical reaction on a metal surface.

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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. Demonstration of geometric diabatic control of quantum states: K. Sasaki, Y. Nakamura, T. Teraji, T. Oka and K. Kobayashi, Phys. Rev. A **107**, 053113 (2023).

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7. *Anomalous Hall Transport by Optically Injected Isospin Degree of Freedom in Dirac Semimetal Thin Film: Y. Murotani, N. Kanda, T. Fujimoto, T. Matsuda, M. Goyal, J. Yoshinobu, Y. Kobayashi, T. Oka, S. Stemmer and R. Matsunaga, Nano Lett. **24**, 222 (2024).

Inoue group

In 2023, we studied the ion-transporting mechanism of channelrhodopsin C1C2 using time-resolved Raman spectroscopy in collaboration with Prof. Akiyama's laboratory. We clarified that the highly twisted retinal chromophore drives the channel opening. We also successfully converted the function of the outward proton-pumping rhodopsin, PspR, into an inward proton-pumping one by mutating three residues in PspR to mimic those in the natural inward proton-pumping rhodopsin, SzR. This study revealed that the directionality of proton transport in rhodopsins is determined by just a few residues. Furthermore, we identified new rhodopsins homologous to TAT rhodopsin in several marine bacteria and classified them into a new family, TwR. Additionally, we investigated the photoreaction cycle of a new class of outward proton-pumping rhodopsin that binds to antennae 3-OH type carotenoids, previously considered incapable of binding to rhodopsins. Moreover, we reported on the photochemical properties of the Retinal G protein-coupled receptor, a new rhodopsin family with a DSE motif, and the structural dynamics of heliorhodopsin.

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8. Biophysical characterization of microbial rhodopsins with DSE motif: M. D. C. Marín, A. L. Jaffe, P. T. West, M. Konno, J. F. Banfield and K. Inoue, Biophys. Physicobiol. **20**, e201023 (2023).

9. Structural basis for ion selectivity in potassium-selective channelrhodopsins: S. Tajima, Y. S. Kim, M. Fukuda, Y. Jo, P. Y. Wang, J. M. Paggi, M. Inoue, E. F. X. Byrne, K. E. Kishi, S. Nakamura, C. Ramakrishnan, S. Takaramoto, T. Nagata, M. Konno, M. Sugiura, K. Katayama, T. E. Matsui, K. Yamashita, S. Kim, H. Ikeda, J. Kim, H. Kandori, R. O. Dror, K. Inoue, K. Deisseroth and H. E. Kato, Cell **186**, 4325.e26 (2023).

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Hayashi group

After transferring from Tohoku University to the Institute for Solid State Physics in 2023, we spent this year summarizing experiments performed at Tohoku University. Transport phenomena such as heat conduction, electric current, and diffusion are the subjects of non-equilibrium statistical mechanics. There are also transport phenomena in the body, and we specifically focus on axonal transport by motor proteins (kinesin and dynein) in neurons as subjects of mathematics and physics research. Last year, we performed fluorescence imaging of axonal transport in neurons of *C. elegans* worms at Tohoku University. We measured the transport velocity data from the recorded movies of the fluorescence imaging. This year, we analyzed the transport velocity of axonal transport obtained last year using extreme value statistics [1]. Applying extreme value statistics to nanoscale biological systems is novel, and we presented the results at a research meeting at the Institute of Statistical Mathematics on

† Joint research with outside partners.

"Applications of Extreme Value Theory in Engineering," discussing the validity of its application. Mutations in motor proteins can lead to axonal transport disorders, leading to the death of neurons and associated with neurological diseases [3]. We presented the results of our lab's physical measurements at the annual meeting of the Japan Neuroscience Society, aiming to elucidate the mechanisms of neurological diseases. Because it's important for doctors, patients, and researchers to consider these issues together, the discussions with doctors at the annual meeting were fruitful. Motor protein research is actively conducted in the United States, so to deepen academic exchange with the US, we organized a joint Japan-US symposium at the Japan Society for Biophysics [2]. Additionally, we gave an oral presentation at the Biophysical Society (USA) annual meeting.

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2. 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).

3. Number of kinesins engaged in axonal cargo transport: A novel biomarker for neurological disorders: K. Hayashi and K. Sasaki, Neuroscience Research **197**, 25-30 (2023).

Quantum Materials Group

Oshikawa group

We have reformulated the Kennedy-Tasaki duality mapping, which was originally proposed in 1992, based on the modern understanding of the Symmetry-Protected Topological (SPT) phases. The duality maps between a SPT phase and a Spontaneous Symmetry Breaking (SSB) phase; a non-local "string" order parameter is mapped to a conventional correlation function of a local order parameter. Although it was originally defined only on open chains, we have generalized it to closed chains as a non-invertible transformation. Applying our reformulated version of the duality to various simple systems, we have constructed numerous SPT phases systematically, including new types of "gapless SPT" phases.

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2. Duality, criticality, anomaly, and topology in quantum spin-1 chains: H. Yang, L. Li, K. Okunishi and H. Katsura, Phys. Rev. B **107**, 125158 (2023).

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7. Fermionization of fusion category symmetries in 1+1 dimensions: K. Inamura, JHEP **2023**, 101(1-63) (2023).

8. Symmetry TFTs and anomalies of non-invertible symmetries: J. Kaidi, E. Nardoni, G. Zafrir and Y. Zheng, JHEP **2023**, 53 (2023).

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10. †*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).

Nakatsuji group

The myths of quantum mechanics render electronic, magnetic, and optical properties in materials that defy common sense while inspiring future technologies. Through decades of effort, researchers studying quantum materials have uncovered a wealth of fascinating properties, ranging from superconductivity that allows electric current to flow without any resistance to topolog-

* Joint research among groups within ISSP.

ical insulators whose surface states serve as superhighways for electrons to flow freely. Discoveries in the field of quantum materials offer a central thread linking the previously disparate fields, like condensed matter physics, high-energy physics, quantum computing, and cosmology. Moreover, the functionalities of quantum materials provide the basis for emerging transformational technologies, such as antiferromagnetic memory. Our vision is to lead the quest for functional quantum materials to bear a groundbreaking impact on fundamental science and benefit humanity in the future. The main research topics in our group are (1) Quantum transport in topological materials; (2) Coherent quantum transport in antiferromagnetic spintronics; (3) Strange metal and exotic superconductivity in strongly correlated electron systems; (4) Long-range quantum entanglement in topologically ordered states.

1. *Ultrafast Dynamics of Intrinsic Anomalous Hall Effect in the Topological Antiferromagnet Mn_3Sn: T. Matsuda, T. Higo, T. Koretsune, N. Kanda, Y. Hirai, H. Peng, T. Matsuo, N. Yoshikawa, R. Shimano, S. Nakatsuji and R. Matsunaga, Phys. Rev. Lett. **130**, 126302 (2023).

2. *High-resolution magnetic imaging by mapping the locally induced anomalous Nernst effect using atomic force microscopy: N. Budai, H. Isshiki, R. Uesugi, Z. Zhu, T. Higo, S. Nakatsuji and Y. Otani, Appl. Phys. Lett. **122**, 102401 (2023).

3. *Octupole-driven magnetoresistance in an antiferromagnetic tunnel junction: X. Chen, T. Higo, K. Tanaka, T. Nomoto, H. Tsai, H. Idzuchi, M. Shiga, S. Sakamoto, R. Ando, H. Kosaki, T. Matsuo, D. Nishio-Hamane, R. Arita, S. Miwa and S. Nakatsuji, Nature **613**, 490-495 (2023).

4. *Temperature-induced anomalous magnetotransport in the Weyl semimetal Mn_3Ge: M. Wu, K. Kondou, T. Chen, S. Nakatsuji and Y. Otani, AIP Advances **13**, 045102 (2023).

5. *Fabrication of single-crystalline $YFeO_3$ films with large antiferromagnetic domains: C. Wang, M. Lippmaa and S. Nakatsuji, J. Appl. Phys. **135**, 113901 (1-8) (2024).

Miwa group

This year we have worked on the following topics: (1) chirality-induced spin selectivity in the absence of bias current, (2) tunneling magnetoresistance using the chiral antiferromagnet Mn_3Sn, and (3) interfacial magnetic anisotropy of the Fe/MgO system. In topic (1), we have summarized our recent work and published a review paper (J. Magn. Magn. Mater. **585**, 171157. In topic (2) we find a novel tunneling magnetoresistance effect in an all antiferromagnetic Mn_3Sn/MgO/Mn_3Sn junction. This is a collaboration work with the groups of Nakatsuji and Otani (Nature **613**, 490). In topic (3), we find that among various alkali halides, fluoride insertion is effective in enhancing the perpendicular magnetic anisotropy of the Fe/MgO system (Phys. Rev. B **107**, 094420).

1. Magnetic anisotropy of Fe/MgO interfaces inserted with alkali halide layers: J. Chen, S. Sakamoto, H. Kosaki and S. Miwa, Phys. Rev. B **107**, 094420 (2023).

2. *Octupole-driven magnetoresistance in an antiferromagnetic tunnel junction: X. Chen, T. Higo, K. Tanaka, T. Nomoto, H. Tsai, H. Idzuchi, M. Shiga, S. Sakamoto, R. Ando, H. Kosaki, T. Matsuo, D. Nishio-Hamane, R. Arita, S. Miwa and S. Nakatsuji, Nature **613**, 490-495 (2023).

3. Observation of large spin conversion anisotropy in bismuth: N. Fukumoto, R. Ohshima, M. Aoki, Y. Fuseya, M. Matsushima, E. Shigematsu, T. Shinjo, Y. Ando, S. Sakamoto, M. Shiga, S. Miwa and M. Shiraishi, Proceedings of the National Academy of Sciences **102**, e2215030120 (2023).

4. Influence of alkali-fluoride insertion layers on the perpendicular magnetic anisotropy at the Fe/MgO interface: J. Chen, S. Sakamoto and S. Miwa, Phys. Rev. B **109**, 064413 (2024).

5. Spontaneous spin selectivity in chiral molecules at the interface: K. Kondou, S. Miwa and D. Miyajima, Journal of Magnetism and Magnetic Materials **585**, 171157 (2023).

Materials Design and Characterization Laboratory

Hiroi group

The nodal-line semimetals NaAlSi and NaAlGe have significantly different ground states despite having similar electronic structures: NaAlSi exhibits superconductivity below 7 K, while NaAlGe exhibits semiconductive electrical conductivity at low temperatures, indicating the formation of a pseudogap at approximately 100 K. The origin of the pseudogap in NaAlGe is unknown but may be associated with excitonic instability. We investigated hole-doping effects on the ground state in the solid solution Na(Al1–xZnx)Ge and discovered that the pseudogap is suppressed continuously with increasing Zn content, followed

† Joint research with outside partners.

by the appearance of a superconducting dome with the highest transition temperature of 2.8 K. This superconductivity most likely results from excitonic fluctuations.

1. †*Fermi surface and light quasi particles in hourglass nodal chain metal β-ReO_2: D. Hirai, T. Anbai, T. Konoike, S. Uji, Y. Hattori, T. Terashima, H. Ishikawa, K. Kindo, N. Katayama, T. Oguchi and Z. Hiroi, J. Phys.: Condens. Matter **35**, 405503 (2023).

2. Anomalous Diamagnetic Torque Signals in Topological Nodal-Line Semimetal NaAlSi: S. Uji, T. Konoike, Y. Hattori, T. Terashima, T. Oguchi, T. Yamada, D. Hirai, T. Ikenobe and Z. Hiroi, J. Phys. Soc. Jpn. **92**, 074703 (2023).

3. *Large magnetic-field-induced strains in sintered chromium tellurides: Y. Kubota, Y. Okamoto, T. Kanematsu, T. Yajima, D. Hirai and K. Takenaka, Appl. Phys. Lett. **122**, 042404 (2023).

4. Superconductivity induced by doping holes in the nodal-line semimetal NaAlGe: T. Ikenobe, T. Yamada, D. Hirai, H. Yamane and Z. Hiroi, Phys. Rev. Materials **7**, 104801 (2023).

5. Nonmagnetic Ground State in RuO2 Revealed by Muon Spin Rotation: M. Hiraishi, H. Okabe, A. Koda, R. Kadono, T. Muroi, D. Hirai and Z. Hiroi, Phys. Rev. Lett. **132**, 166702 (2024).

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 2023: (1) Classical spin systems with novel phase transitions and excitations [Okubo and Kawashima, JPSJ92; Tu, et al, PRB107; Watanabe, et al, PTP2023, PRR5], (2) Data-scientific approach to material design [Kavacs, et al, Front.Mater.9], (3) Development of open-source software for condensed matter calculations [Kurita, CPC292], (4) Down-folding method for strongly correlated electron systems such as superconductors [Ido, et al, JPSJ92]

1. *Data Analysis of Ab initio Effective Hamiltonians in Iron-Based Superconductors — Construction of Predictors for Superconducting Critical Temperature: K. Ido, Y. Motoyama, K. Yoshimi and T. Misawa, J. Phys. Soc. Jpn. **92**, 064702(1-13) (2023).

2. Possibility of a Topological Phase Transition in Two-dimensional RP3 Model: T. Okubo and N. Kawashima, J. Phys. Soc. Jpn. **92**, 114701 (2023).

3. Cubic ferromagnet and emergent U(1) symmetry on its phase boundary: W.-L. Tu, X. Lyu, S. R. Ghazanfari, H.-K. Wu, H.-Y. Lee and N. Kawashima, Phys. Rev. B **107**(1-14) (2023).

4. *Interface tool from Wannier90 to RESPACK: wan2respack: K. Kurita, T. Misawa, K. Yoshimi, K. Ido and T. Koretsune, Comput. Phys. Commun. **292**, 108854(1-7) (2023).

5. Non-monotonic behavior of the Binder parameter in discrete spin systems: H. Watanabe, Y. Motoyama, S. Morita and N. Kawashima, Prog. Theor. Exp. Phys. **2023**, 033A02 (2023).

6. Ashkin-Teller phase transition and multicritical behavior in a classical monomer-dimer model: S. Morita, H.-Y. Lee, K. Damle and N. Kawashima, Physical Review Research **5**, 043061(1-12) (2023).

7. Physics-informed machine learning combining experiment and simulation for the design of neodymium-iron-boron permanent magnets with reduced critical-elements content: A. Kovacs, J. Fischbacher, H. Oezelt, A. Kornell, Q. Ali, M. Gusenbauer, M. Yano, N. Sakuma, A. Kinoshita, T. Shoji, A. Kato, Y. Hong, S. Grenier, T. Devillers, N. M. Dempsey, T. Fukushima, H. Akai, N. Kawashima, T. Miyake and T. Schrefl, Front. Mater. **9**, 1094055 (2023).

8. †*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).

9. †*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).

Uwatoko group

MnP is found to be superconducting below ~ 1 K around 8 GPa. To elucidate the magnetic ground state adjacent to the superconducting phase first discovered in Mn-based materials, high-pressure neutron diffraction measurements have been performed at hydrostatic pressures up to 7.5 GPa. Combining the experimental and theoretical results, the details of exchange interactions

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* Joint research among groups within ISSP.

in the vicinity of the superconducting phase are described, which is critical to understanding the pairing mechanism of the unconventional superconductivity in MnP. The study of the iron-based superconductor, FeSe, has resulted in various interesting topics. We present the observation of spin fluctuations originating from Bogoliubov Fermi surfaces in the superconducting state via ^{77}Se-nuclear magnetic resonance measurements to 100 mK. In S-substituted FeSe, an abnormal enhancement of low-energy spin uctuations deep in the SC state is established, which cannot be explained by an impurity effect. The recently discovered CsV_3Sb_5 is a new family of kagome superconductors with the superconducting transition temperature Tc of 2.5 K. Our results support that material is a non-chiral, anisotropic s-wave superconductor with no sign change both at ambient and under pressure. $CeNiC_2$ features unique properties such as heavy fermionic behavior and multiple magnetic ordering. With applying pressure, a superconducting dome with a maximum Tc ~ 3.5 K emerges in a narrow pressure range of around 11 GPa. We investigate its crystal structure from ambient pressure to 18.6 GPa via single crystal x-ray diffraction. The pressure dependence of unit-cell parameters reveals anisotropic linear compressibility κ, following $|\kappa_a|$ (3.70×10^{-3} GPa^{-1}) > $|\kappa_c|$ (1.97×10^{-3} GPa^{-1}) > $|\kappa_b|$ (1.39×10^{-3} GPa^{-1}), and a bulk modulus, B_0 ~ 134 ± 3 GPa. The directions of the first nearest and the second nearest neighbors between both the Ce-Ce and Ni-Ni atoms switch at ~ 7 GPa. The 12442-type hybrid structure compound $BaTh_2Fe_4As_4(Na_{0.7}O_{0.3})_2$ shows the superconducting transition at T_c^{onset} ~ 30 K and T_c^{zero} ~ 20 K. We found that T_c(P) exhibits a nonmonotonic variation with pressure, forming a dome-shaped superconducting temperature at optimal values of ~ 46 K at 2.6 GPa. We have measured the high-pressure experiments of $La_3Ni_2O_7$ polycrystalline samples. The constructed T-P phase diagram shares similar features with that of $La_3Ni_2O_7$ crystals and reveals the close relationship between superconductivity, density wave order, and strange-metal-like behavior in this system.

1. Pressure-induced linear enhancement of the superconducting transition in $Nd_{0.8}Sr_{0.2}NiO_2$ thin films: N. N. Wang, G. Wang, Q. Gao, K. Y. Chen, J. Hou, X. L. Ren, Y. Uwatoko, B. S. Wang, Z. H. Zhu, J. P. Sun and J.-G. Cheng, J. Phys.: Condens. Matter **36**, 125601(1-6) (2023).

2. Destabilization of Excitonic Phase by Elemental Substitution in $(Ta_{1-x}M_x)_2NiSe_5$(M=V, Nb) and $Ta_2(Ni_{1-y}T_y)Se_5$(T= Fe, Co): Y. Hirose, S. Sano, T. Hirahara, Y. Uwatoko, J. Gouchi, T. Takeuchi and R. Settai, J. Phys. Soc. Jpn. **92**, 084705(1-7) (2023).

3. Pressure-induced Structural Phase Transition and New Superconducting Phase in UTe_2: F. Honda, S. Kobayashi, N. Kawamura, S. I. Kawaguchi, T. Koizumi, Y. J. Sato, Y. Homma, N. Ishimatsu, J. Gouchi, Y. Uwatoko, H. Harima, J. Flouquet and D. Aoki, J. Phys. Soc. Jpn. **92**, 044702(1-10) (2023).

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5. Atomic coordinates of $CeNiC_2$ under pressure: Switching of the Ce-Ce first nearest neighbor direction: H. Ma, D. Bhoi, J. Gouchi, H. Sato, T. Shigeoka, J. -G. Cheng and Y. Uwatoko, Phys. Rev. B **108**, 064435(1-6) (2023).

6. Complex evolution of the magnetic transitions and unexpected absence of bulk superconductivity in chemically precompressed $NaMn_6Bi_5$: P. F. Shan, Q. X. Dong, P. T. Yang, L. Xu, Z. Y. Liu, L. F. Shi, N. N. Wang, J. P. Sun, Y. Uwatoko, G. F. Chen, B. S. Wang and J. -G. Cheng, Phys. Rev. B **107**, 094519(1-7) (2023).

7. Effect of hydrostatic pressure on the unconventional charge density wave and superconducting properties in two distinct phases of doped kagome superconductors $CsV_{3-x}Ti_xSb_5$: J. Hou, K. Y. Chen, J. P. Sun, Z. Zhao, Y. H. Zhang, P. F. Shan, N. N. Wang, H. Zhang, K. Zhu, Y. Uwatoko, H. Chen, H. T. Yang, X. L. Dong, H. -J. Gao and J. -G. Cheng, Phys. Rev. B **107**, 144502(1-8) (2023).

8. Pressure-driven evolution of upper critical field and Fermi surface reconstruction in the strong-coupling superconductor Ti_4Ir_2O: L. Shi, B. Ruan, P. Yang, N. Wang, P. Shan, Z. Liu, J. Sun, Y. Uwatoko, G. Chen, Z. Ren, B. Wang and J. Cheng, Phys. Rev. B **107**, 174525(1-7) (2023).

9. *Piston-cylinder cell made of Ni–Cr–Al alloy for magnetic susceptibility measurements under high pressures in pulsed high magnetic fields: K. Nihongi, T. Kida, Y. Narumi, N. Kurita, H. Tanaka, Y. Uwatoko, K. Kindo and M. Hagiwara, Rev. Sci. Instrum. **94**, 113903(1-7) (2023).

10. Mgnetic ground state of $YbCo_2Zn_{20}$ probed by muon spin relaxation: W. Higemoto, K. Satoh, T. U. Ito, K. Ohishi, Y. Saiga, M. Kosaka, K. Matsubayashi and Y. Uwatoko, J. Phys.: Conf. Ser. **2462**, 012039(1-5) (2023).

11. Pressure-enhanced superconducting transition in the inter-block-layer electron-transfer superconductor $BaTh_2Fe_4As_4(N_{0.7}O_{0.3})_2$: P. Shan, P. Yang, Y. Shao, Z. Liu, J. Hou, B. Wang, Y. Uwatoko, G. Cao, J. Sun and J. Cheng, Phys. Rev. Materials **7**, 124801(1-8) (2023).

12. Bulk evidence of anisotropic s-wave pairing with no sign change in the kagome superconductor CsV_3Sb_5: M. Roppongi, K. Ishihara, Y. Tanaka, K. Ogawa, K. Okada, S. Liu, K. Mukasa, Y. Mizukami, Y. Uwatoko, R. Grasset, M. Konczykowski, B. R. Ortiz, S. D. Wilson, K. Hashimoto and T. Shibauchi, Nat Commun **14**, 667(1-8) (2023).

13. *Helical magnetic state in the vicinity of the pressure-induced superconducting phase in MnP: S. E. Dissanayake, M.

† Joint research with outside partners.

Matsuda, K. Yoshimi, S. Kasamatsu, F. Ye, S. Chi, W. Steinhardt, G. Fabbris, S. Haravifard, J. Cheng, J. Yan, J. Gouchi and Y. Uwatoko, Phys. Rev. Research **5**, 043026(1-13) (2023).

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15. Emergence of High-Temperature Superconducting Phase in Pressurized $La_3Ni_2O_7$ Crystals: J. Hou, P.-T. Yang, Z.-Y. Liu, J.-Y. Li, P.-F. Shan, L. Ma, G. Wang, N.-N. Wang, H.-Z. Guo, J.-P. Sun, Y. Uwatoko, M. Wang, G.-M. Zhang, B.-S. Wang and J.-G. Cheng, Chinese Phys. Lett. **40**, 117302(1-6) (2023).
16. Pressure-induced Superconductivity in BiS_2-based Superconductors $Eu_2SrBi_2S_{2.5}Se_{1.5}F_4$: 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).
17. From semiconductor to Fermi metal and emergent density-wave-like transition in the quasi-one-dimensional *n*-type $Bi_{19}S_{27}I_3$ under hydrostatic pressure: S. Xu, Z. Liu, P. Yang, B. Ruan, Z. Ren, J. Sun, Y. Uwatoko, B. Wang and J. Cheng, Phys. Rev. B **109**, 144107(1-10) (2024).
18. Quantum criticality in $YbCu_4Ni$: 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).
19. Pressure-Induced Superconductivity In Polycrystalline $La_3Ni_2O_{7-\delta}$: G. Wang, N. N. Wang, X. L. Shen, J. Hou, L. Ma, L. F. Shi, Z. A. Ren, Y. D. Gu, H. M. Ma, P. T. Yang, Z. Y. Liu, H. Z. Guo, J. P. Sun, G. M. Zhang, S. Calder, J. Q. Yan, B. S. Wang, Y. Uwatoko and J. -G. Cheng, Phys. Rev. X **14**, 011040(1-8) (2024).
20. Pressure Effect on the Magnetic Properties of the Heusler Alloy Co_2NbGa: Y. Adachi, Y. Ogi, T. Osaki, T. Eto, T. Kihara, H. Nishihara, T. Sakon, J. Gouchi, Y. Uwatoko and T. Kanomata, J Supercond Nov Magn **37**, 249-254 (2024).

Ozaki group

For more than last 5 years, we have been collaborating with the Sugimoto laboratory in the graduate school of frontier sciences, the University of Tokyo to unveil surface structures and their electronic structures of silicene and diamond surface, which have been investigated by scanning tunneling microscopy (STM) and atomic force microscopy (AFM). Our role in the collaboration is to theoretically understand their experimental observation by making use of first-principles calculations. We have established computational schemes to calculate the force spectroscopy, in which perpendicular forces acting on model tips consisting of silicon atoms and the surfaces are directly calculated, and compared calculated force spectroscopy data with the experimental data. The comparison leads to excellent agreement with the experimentally data not only qualitatively and but also quantitatively. In the fiscal year, our special focus was to investigate detailed structures of Si adatoms on silicene on Ag(111) surface and the surface structures of diamond(001). These studies provided clear pictures for the thermodynamic energetics of the surface structures, and an evidence that the high resolution of AFM image in the experiments should be attributed to bond formation between the tip and surface atoms which is far from the non-contact regime.

1. †*Ambipolar Nickel Dithiolene Complex Semiconductors: From One- to Two-Dimensional Electronic Structures Based upon Alkoxy Chain Lengths: M. Ito, T. Fujino, L. Zhang, S. Yokomori, T. Higashino, R. Makiura, K. J. Takeno, T. Ozaki and H. Mori, J. Am. Chem. Soc. **145**, 2127-2134 (2023).
2. †*Metallic State of a Mixed-Sequence Oligomer Salt That Models Doped PEDOT Family: K. Onozuka, T. Fujino, R. Kameyama, S. Dekura, K. Yoshimi, T. Nakamura, T. Miyamoto, T. Yamakawa, H. Okamoto, H. Sato, T. Ozaki and H. Mori, J. Am. Chem. Soc. **145**, 15152-15161 (2023).
3. Atomically thin metallic Si and Ge allotropes with high Fermi velocities: C. -E. Hsu, Y. -T. Lee, C. -C. Wang, C. -Y. Lin, Y. Yamada-Takamura, T. Ozaki and C. -C. Lee, Physical Review B **107**, 115410 (2023).
4. Atomic arrangement of Si adatom on the Silicene/Ag (111) surface: Y. Adachi, R. Zhang, X. Wang, M. Fukuda, T. Ozaki and Y. Sugimoto, Applied Surface Science **630**, 157336 (2023).
5. *Hydrogen - induced Sulfur Vacancies on the MoS_2 Basal Plane Studied by Ambient Pressure XPS and DFT Calculations: F. Ozaki, S. Tanaka, Y. Choi, W. Osada, K. Mukai, M. Kawamura, M. Fukuda, M. Horio, T. Koitaya, S. Yamamoto, I. Matsuda, T. Ozaki and J. Yoshinobu, ChemPhysChem **24**, e202300477 (2023).

Noguchi group

We have studied (1) microphase separation with checkerboard and kagome lattice patterns induced by the binding of curvature-

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inducing proteins onto both sides of a membrane, (2) excitable waves on a deformable membrane tube, (3) estimation of anisotropic bending coefficients of crescent proteins from experimental data, and (4) the effects of interfacial tension of phase boundary on membrane rupture.

1. Phase-Separated Giant Liposomes for Stable Elevation of α-Hemolysin Concentration in Lipid Membranes: M. Kobayashi, H. Noguchi, G. Sato, C. Watanabe, K. Fujiwara and M. Yanagisawa, Langmuir **39**, 11481-11489 (2023).

2. Estimation of anisotropic bending rigidities and spontaneous curvatures of crescent curvature-inducing proteins from tethered-vesicle experimental data: H. Noguchi, N. Walani and M. Arroyo, Soft Matter **19**, 5300-5310 (2023).

3. Membrane domain formation induced by binding/unbinding of curvature-inducing molecules on both membrane surfaces: H. Noguchi, Soft Matter **19**, 679-688 (2023).

4. Disappearance, division, and route change of excitable reaction-diffusion waves in deformable membranes: H. Noguchi, Sci Rep **13**, 6207(1-8) (2023).

5. Curvature sensing of curvature-inducing proteins with internal structure: H. Noguchi, Phys. Rev. E **109**, 024403/1-10 (2024).

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 2023 include functional and usability enhancement of (1) TeNeS and making new tools (2) cif2x and Moller. We published five papers about the developed software packages (abICS,H-wave, and Hφ) in PASUMS. In addition, using the software packages developed by PASUMS, we have studied electronic properties of organic conductors such as α-(BEDT-TTF)$_2$I$_3$, α-(BEDT-TSeF)$_2$I$_3$, and TM salts.

1. *Data Analysis of Ab initio Effective Hamiltonians in Iron-Based Superconductors — Construction of Predictors for Superconducting Critical Temperature: K. Ido, Y. Motoyama, K. Yoshimi and T. Misawa, J. Phys. Soc. Jpn. **92**, 064702(1-13) (2023).

2. †*Gap opening mechanism for correlated Dirac electrons in organic compounds α-(BEDT−TTF)$_2$I$_3$ and α-(BEDT−TSeF)$_2$I$_3$: D. Ohki, K. Yoshimi, A. Kobayashi and T. Misawa, Phys. Rev. B **107**, L041108(1-6) (2023).

3. †*Comprehensive Ab Initio Investigation of the Phase Diagram of Quasi-One-Dimensional Molecular Solids: K. Yoshimi, T. Misawa, T. Tsumuraya and H. Seo, Phys. Rev. Lett. **131**, 036401(1-7) (2023).

4. †*Metallic State of a Mixed-Sequence Oligomer Salt That Models Doped PEDOT Family: K. Onozuka, T. Fujino, R. Kameyama, S. Dekura, K. Yoshimi, T. Nakamura, T. Miyamoto, T. Yamakawa, H. Okamoto, H. Sato, T. Ozaki and H. Mori, J. Am. Chem. Soc. **145**, 15152-15161 (2023).

5. †*Precise Control of the Molecular Arrangement of Organic Semiconductors for High Charge Carrier Mobility: R. Akai, K. Oka, S. Dekura, K. Yoshimi, H. Mori, R. Nishikubo, A. Saeki and N. Tohnai, J. Phys. Chem. Lett. **14**, 3461 (2023).

6. *Interface tool from Wannier90 to RESPACK: wan2respack: K. Kurita, T. Misawa, K. Yoshimi, K. Ido and T. Koretsune, Comput. Phys. Commun. **292**, 108854(1-7) (2023).

7. *Helical magnetic state in the vicinity of the pressure-induced superconducting phase in MnP: S. E. Dissanayake, M. Matsuda, K. Yoshimi, S. Kasamatsu, F. Ye, S. Chi, W. Steinhardt, G. Fabbris, S. Haravifard, J. Cheng, J. Yan, J. Gouchi and Y. Uwatoko, Phys. Rev. Research **5**, 043026(1-13) (2023).

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9. †Configuration sampling in multi-component multi-sublattice systems enabled by ab Initio Configuration Sampling Toolkit (abICS): S. Kasamatsu, Y. Motoyama, K. Yoshimi and T. Aoyama, Science and Technology of Advanced Materials: Methods **3**, 2284128 (2023).

10. †*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).

11. †*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).

12. †*H-wave – A Python package for the Hartree-Fock approximation and the random phase approximation: T. Aoyama, K.

† Joint research with outside partners.

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13. †*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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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 Sc_6MTe_2, Zr_6MTe_2, ScPdGe, and ScPdSi, where M is transition metal elements, and a frustrated spin system $NaLnTe_2$. In these materials, Sc_6MTe_2 is a unique *d*-electron superconducting family incorporating 3*d*, 4*d*, and 5*d* electrons systems. The critical temperatures T_c for M = 3*d* elements are higher than those for 4*d* and 5*d* elements and increase in the order of M = Ni, Co, and Fe with the highest T_c of 4.7 K in Sc_6FeTe_2, suggesting that the Fe 3*d* electrons play important roles in realizing the highest T_c. On the other hand, Sc_6OsTe_2 and Sc_6IrTe_2 show a superconductivity with a high upper critical field H_{c2} violating the Pauli limit, caused by the strong spin-orbit coupling of Os and Ir 5*d* electrons. It is rare that such 3*d* and 5*d* electron features play major roles in an isostructural *d*-electron superconductor family.

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Yamaura group

Our laboratory started in 2023, and this year we used quantum beams to determine the structures of various materials from basic to applied sciences, including magnetic nanowires, novel ferroelectrics, novel high dielectrics, novel thermoelectric materials, magnetic thin films, nodal line semimetals, and more. Moreover, the joint use operation of the X-Ray Diffraction Section at the Materials Design and Characterization Laboratory (MDCL) is progressing smoothly, providing not only user support to various users inside and outside the institute, but also analytical advice, new research proposals, and even paths to 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.

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Neutron Science Laboratory

Yamamuro group

Our laboratory is studying chemical physics of complex condensed matters by using neutron scattering, X-ray diffraction, calorimetric, dielectric, and viscoelastic techniques. Our target materials are glasses, liquids, and various disordered systems. In 2023, we have measured the heat capacities of vapor-deposited H_2O and CS_2 by using a custom-made adiabatic calorimeter. Their heat capacities were consistent with the inelastic neutron scattering data obtained before. We have also measured the X-ray (BL04B2@SPring-8) and neutron (BL21@J-PARC) diffractions and quasielastic neutron scattering (AGNES@JRR-3) data of vapor-deposited amorphous methane hydrate. These data revealed that methane molecules are accommodated in cage-like spaces in an amorphous structure, and they exhibit a classical rotation at higher temperatures and a quantum (tunneling) rotation at lower temperatures. The quasielastic neutron scattering using AGNES@JRR-3 and BL02@J-PARC were conducted also for a typical metal-organic framework MOF-101 including acetonitrile molecules and $Mg(TFSI)_2$ in the pores. This material is a good candidate of future solid batteries because of its higher volumetric capacity than lithium-ion batteries and the abundancy of Mg. The motion of acetonitrile molecules was quite high, being associated with the high mobility of Mg ions.

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Masuda group

The goal of our research is to discover a new quantum phenomenon and to reveal the mechanism of it. In this fiscal year we studied the following topics; Inelastic neutron scattering in the weakly coupled triangular spin tube candidate $CsCrF_4$, Magnetic structure of the magnetoelectric material $Ba_2MnGe_2O_7$, Spin excitation in the coupled honeycomb lattice compound Ni_2InSbO_6, Magnetic Resonance in the Quasi-2D Square Lattice Easy-Plane Antiferromagnet $Ba_2MnGe_2O_7$, and so on.

† Joint research with outside partners.

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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 also responsible for a polarized-neutron triple-axis neutron spectrometer PONTA in the research reactor JRR-3 in Tokai, which restarted in 2021 after the long shutdown since the east Japan great earthquake in 2011. As the instrument team of PONTA, we have been supporting the users of the joint-use program, and have collaborated in their researches. One of the successful experiments at PONTA in the fiscal year of 2023 is the observation of the incommensurate magnetic modulation associated the charge density wave in UPt_2Si_2. Prof. Amitsuka's group in the Hokkaido university grew single crystal of this compound, which was known to exhibit a commensurate antiferromagnetic (AF) order and incommensurate charge density wave (CDW). They found that the commensurate AF order was affected by the CDW, and that the incommensurate magnetic modulations appear below the transition temperature. By utilizing the polarized neutron scattering technique, they successfully observed incommensurate magnetic reflections appearing at the same position as nuclear superlattice reflection associated with the CDW. Nakajima group is also working on developing new neutron scattering techniques in extreme conditions. Since 2019, we have been collaborating with Prof. Kohama's group in IMGSL of ISSP to realize stroboscopic neutron diffraction in long pulsed magnetic fields. We recently employed this technique to explore field induced magnetic phases in a triangular lattice antiferromagnet $CuFe_{1-x}Ga_xO_2$. We are planning to apply this technique to various magnetic materials in the future.

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Mayumi group

For separator membranes of flexible batteries, mechanical stiffness (high Young's modulus) and toughness (high fracture energy) are required. Mayumi group has successfully developed tough and stiff ion gels using phase separation and strain-induced crystallization. In addition, we have investigated network structure of polysaccaride hydrogels for food applications by using SANS. The rigidity and size of chain aggregates dominate their macroscopic rheological properties.

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† Joint research with outside partners.

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International MegaGauss Science Laboratory

Kindo group

A better Cu-Ag magnet wire was developed. Our mono-coil renewed the world record of the non-destructive pulsed field. 88.6 T was generated by using the new Cu-Ag wire.

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In the quantum limit state realized in high field limit, we can increase the effect of electron correlation by applied magnetic fields. In our study on BiSb alloys, we induced transitions from topological insulator to topologically non-trivial semimetal by magnetic fields applied along the trigonal axis. In addition, we found the system changes into insulator again by further increasing applied field in the quantum limit state of the field-induced semimetallic state. We discussed possibility of the excitonic insulator state that has been anticipated over half a century.

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Y. Matsuda group

We have investigated magnetic states in several frustrated spin systems such as breathing pyrochlore, Kitaev, and Shastry-Sutherland systems with ultrahigh-magnetic fields exceeding 100 T. In the breathing pyrochlore systems, the strong spin-lattice coupling was found to be important. The magnetic field-induced quantum spin liquid state appeared in a Kitaev system $RuCl_3$ when the field was perpendicular to the honeycomb plane, which was in good agreement with a theoretical calculation. An unusual decrease in the sound velocity was observed at the 1/2 plateau in the Shastry-Sutherland system $SrCu_2(BO_3)_2$ in addition to the success of having a saturation at around 140 T. The electronic structure in a functional semiconductor $In_{1-x}As_xP$ has been revealed by using cyclotron resonance in magnetic fields of up to 140 T. The strongly correlated transition metal perovskite oxides, $Bi_{0.5}Ca_{0.5}MnO_3$ and $LaCoO_3$ were also studied. The charge order in $Bi_{0.5}Ca_{0.5}MnO_3$ gradually melts with the increasing magnetic field, while the re-order occurs rather sharply, which indicates an interesting metastable state that appears in magnetic fields fastly varying with time. As for $LaCoO_3$, the quantum condensed exciton state is indicated at ultra-high magnetic fields up to 600 T. The spin-state transition with a strong quantum entanglement occurs in the ultrahigh magnetic fields.

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We have investigated high-field properties on various compounds. In magnetic materials, such as $CuGaCr_4S_8$, Sr(TiO)$Cu_4(PO_4)_4$, $LiGaCr_4O_8$, and $SrCu_2(BO_3)_2$, the field-induced phase transitions have been investigated by magnetization and thermodynamic experiments using non-destructive and destructive magnetic fields. In two dimensional conductors, graphite, high-Tc cuprates, and Iron based superconductors, we have investigated the quantum transport properties. Here, the TDO, torque magnetometry, and specific heat measurements have revealed rich quantum phenomena. We have also succesfully develop rf transport measurement technique and field generatoin technique for further detailed investigations in high magnetic fields.

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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 van der Waals magnets. The vdW magnet FePS3, which has a zigazag magnetic order below TN ~ 120 K, exhibits giant linear dichroism, i.e., linearly polarized lights parallel and perpendicular to the zigzag chain direction show different responses. Magnetic fields can quench the giant linear dichroism in a wide energy range from 1.6 to 2.0 eV by collapsing the robust zigzag magnetic order.

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), released H-wave (software for Hartree-Fock calculations and random phase approximations), and wan2respack (an interface tool from Wannier90 to RESPACK). Using these software packages, we have performed ab initio calculations for molecular solids, such as TMTTF/TMTSF salts.

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Laser and Synchrotron Research Center

Kobayashi group

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Harada group

In 2023, we made significant progress in the analysis of single crystalline $LiFe_{0.6}Mn_{0.4}PO_4$ (LFMP) nanowires with carbon sheath using scanning transmission X-ray microscopy (STXM) with a spatial resolution of around 130 nm. The pinpoint Fe *L*-edge and O *K*-edge X-ray absorption spectroscopy (XAS) spectra revealed the natural oxidation of Fe^{2+} to Fe^{3+} near the tip of the nanowire by air exposure, while the Mn *L*-edge XAS spectra showed a stable Mn^{2+} state throughout the nanowires. We also investigated the spatial distributions of the chemical states in prototypical layered $LiCoO_2$ cathode particles at different charging conditions using STXM. The Co LL_3- and O *K*-edge XAS spectra demonstrated the spatial distribution of the chemical state changes depending on individual particles, and the element maps derived from the STXM stack images revealed the inhomogeneous reactions and the existence of non-active particles. Furthermore, we applied microscopic resonant photoelectron spectroscopy with a spatial resolution of 100 nm (3DnanoESCA system) to study the electronic structure of different facets of $LiCoO_2$ cathode particles, detecting differences in the binding energies of the dominant Co 3d bands at the valence band of the (001), (104), and (012) facets. Lastly, we prepared for the operation of the next generation synchrotron radiation facility NanoTerasu starting from April 2024 by setting up the RIXS and 3D nanoESCA stations.

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I. Matsuda group

We have conducted instrumentations at the new synchrotron radiation (SR) facility, NanoTerasu, at Sendai in Miyagi-prefecture. We have updated our experimental station of ambient-pressure X-ray spectroscopy and developed a system of process-informatics robot units. We have also devoted ourselves in supporting the beamline construction. On December 7, 2023, the first beam was successfully achieved in NanoTerasu. Tuning of the SR beam has been carried out at the beamline and at the end-station. At the X-ray free electron laser (XFEL) beamline, SACLA BL-1, we have succeeded in observing the magnetization-induced second harmonic generation. Based on results of the SR and XFEL experiments, we discovered new 2D boron materials and examined the properities.

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Itatani group

* Joint research among groups within ISSP.

We have promoted soft X-ray attosecond spectroscopy by using a thin flat water jet introduced into a newly developed attosecond beamline in collaboration with RIKEN. An optical parametric amplifier was also installed in the beamline for various pump-probe experiments. We have also developed a new optical parametric amplifier in the infrared (wavelength around 2 micrometers) pumped by a compact Yb:KGW laser system at 1030 nm with a repetition rate of 100 kHz. The output pulse duration is 16 fs with an extremely stable carrier-envelope phase. This system is designed as a front-end for future high-power ultrafast light sources for high-throughput attosecond soft-X-ray spectroscopy. We have also pursued the ultrafast strong field phenomena in liquids using a thin flat jet setup with an improved intense MIR source. With the sub-cycle spectroscopy experiment, unusual superluminal propagation of MIR pulses was observed due to strong resonance absorption. High harmonic generation with resonant MIR pulses in water was studied and a novel thermal enhancement was observed for the first time, opening a new direction in strong-field attosecond science in condensed matter.

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† Joint research with outside partners.

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Kondo group

We revealed the semiconducting electronic structure of the ferromagnetic spinel HgCr2Se4 and determined the phase diagram of the lightly doped high-Tc cuprate superconductors with disorder removed via observing six-layered cuprates.

1. *Semiconducting Electronic Structure of the Ferromagnetic Spinel $HgCr_2Se_4$ Revealed by Soft-X-Ray Angle-Resolved Photoemission Spectroscopy: H. Tanaka, A. V. Telegin, Y. P. Sukhorukov, V. A. Golyashov, O. E. Tereshchenko, A. N. Lavrov, T. Matsuda, R. Matsunaga, R. Akashi, M. Lippmaa, Y. Arai, S. Ideta, K. Tanaka, T. Kondo and K. Kuroda, Phys. Rev. Lett. **130**, 186402 (1-6) (2023).

2. *Nodeless electron pairing in CsV3Sb5-derived kagome superconductors: Y. Zhong, J. Liu, X. Wu, Z. Guguchia, J. -X. Yin, A. Mine, Y. Li, S. Najafzadeh, D. Das, C. Mielke, R. Khasanov, H. Luetkens, T. Suzuki, K. Liu, X. Han, T. Kondo, J. Hu, S. Shin, Z. Wang, X. Shi, Y. Yao and K. Okazaki, Nature **617**, 488 (2023).

3. *Testing electron-phonon coupling for the superconductivity in kagome metal CsV_3Sb_5: Y. Zhong, S. Li, H. Liu, Y. Dong, K. Aido, Y. Arai, H. Li, W. Zhang, Y. Shi, Z. Wang, S. Shin, H. N. Lee, H. Miao, T. Kondo and K. Okazaki, Nat. Commun. **14**, 1945 (2023).

4. †*Unveiling phase diagram of the lightly doped high-Tc cuprate superconductors with disorder removed: K. Kurokawa, S. Isono, Y. Kohama, S. Kunisada, S. Sakai, R. Sekine, M. Okubo, M. D. Watson, T. K. Kim, C. Cacho, S. Shin, T. Tohyama, K. Tokiwa and T. Kondo, Nat Commun **14**, 4064 (2023).

5. *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).

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, we have reported ultrafast dynamics of the anomalous Hall effect in a magnet with sub-100 fs time resolution for the first time. We also observed the light-induced anomalous Hall effect in a Dirac semimetal and succeeded in providing classification of the competing mechanisms. Our THz polarimetry technique offers a unique pathway to disentangle the microscopic mechanisms of anomalous transport in solids.

1. *Disentangling the Competing Mechanisms of Light-Induced Anomalous Hall Conductivity in Three-Dimensional Dirac Semimetal: Y. Murotani, N. Kanda, T. Fujimoto, T. Matsuda, M. Goyal, J. Yoshinobu, Y. Kobayashi, T. Oka, S. Stemmer and R. Matsunaga, Phys. Rev. Lett. **131**, 096901 (2023).

2. *Semiconducting Electronic Structure of the Ferromagnetic Spinel $HgCr_2Se_4$ Revealed by Soft-X-Ray Angle-Resolved Photoemission Spectroscopy: H. Tanaka, A. V. Telegin, Y. P. Sukhorukov, V. A. Golyashov, O. E. Tereshchenko, A. N. Lavrov, T. Matsuda, R. Matsunaga, R. Akashi, M. Lippmaa, Y. Arai, S. Ideta, K. Tanaka, T. Kondo and K. Kuroda, Phys. Rev. Lett. **130**, 186402 (1-6) (2023).

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7. *Pump-probe spectroscopy for non-equilibrium condensed matter: R. Matsunaga and K. Okazaki, Encyclopedia of

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Condensed Matter Physics, Second Edition **1**, 981 (2023).

8. *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 (2024).

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11. *Anomalous Hall Transport by Optically Injected Isospin Degree of Freedom in Dirac Semimetal Thin Film: Y. Murotani, N. Kanda, T. Fujimoto, T. Matsuda, M. Goyal, J. Yoshinobu, Y. Kobayashi, T. Oka, S. Stemmer and R. Matsunaga, Nano Lett. **24**, 222 (2024).

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Okazaki group

We have investigated the 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 2023, we have successfully observed the superconducting gap in a pristine sample of the Kagome superconductor CsV_3Sb_5 by high-resolution laser ARPES. In addition, we have successfully observed the pump-wavelength-dependent photoexcited electron dynamics in a rare-earth trichalcogenide material exhibiting a CDW by HHG laser time-resolved ARPES.

1. †*Quasi One-Dimensional Band Structure of Photoinduced Semimetal Phase of $Ta_2Ni_{1-x}Co_xSe_5$ (x = 0.0 and 0.1): T. Mitsuoka, Y. Takahashi, T. Suzuki, M. Okawa, H. Takagi, N. Katayama, H. Sawa, M. Nohara, M. Watanabe, J. Xu, Q. Ren, M. Fujisawa, T. Kanai, J. Itatani, K. Okazaki, S. Shin and T. Mizokawa, J. Phys. Soc. Jpn. **92**, 023703 (2023).

2. †*Temporal Evolution and Fluence Dependence of Band Structure in Photoexcited $Ta_2Ni_{0.9}Co_{0.1}Se_5$ Probed by Time- and Angle-Resolved Photoemission Spectroscopy: Y. Takahashi, T. Suzuki, M. Hattori, M. Okawa, H. Takagi, N. Katayama, H. Sawa, M. Nohara, Y. Zhong, K. Liu, T. Kanai, J. Itatani, S. Shin, K. Okazaki and T. Mizokawa, J. Phys. Soc. Jpn. **92**, 064706 (2023).

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9. *Testing electron-phonon coupling for the superconductivity in kagome metal CsV_3Sb_5: Y. Zhong, S. Li, H. Liu, Y. Dong, K. Aido, Y. Arai, H. Li, W. Zhang, Y. Shi, Z. Wang, S. Shin, H. N. Lee, H. Miao, T. Kondo and K. Okazaki, Nat. Commun. **14**, 1945 (2023).

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10. †*Direct observation of multiple conduction-band minima in high-performance thermoelectric SnSe: M. Okawa, Y. Akabane, M. Maeda, G. Tan, L.-D. Zhao, M. G. Kanatzidis, T. Suzuki, M. Watanabe, J. Xu, Q. Ren, M. Fujisawa, T. Kanai, J. Itatani, S. Shin, K. Okazaki, N. L. Saini and T. Mizokawa, Scripta Materialia **223**, 115081 (2023).

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Kimura group

In FY2023, we developed soft X-ray optics techniques using BL07LSU, which is now owned by RIKEN. In particular, we worked on the construction of a soft X-ray microscope using a total reflection mirror, the development of a lensless imaging technique, the ptychography method, and an ultrafast imaging technique using magnification imaging optics. Using such soft X-ray microscopes, we were engaged in the observation of mouse neurons and pancreatic cells and the development of operando measurement techniques for device evaluation.

1. †* ウォルターミラーを利用した軟 X 線タイコグラフィ装置の開発 : 木村 隆志 , 竹尾 陽子 , 櫻井 快 , 古谷 登 , 江川 悟 , 山口 豪太 , 松澤 雄介 , 久米 健大 , 三村 秀和 , 志村 まり , 大橋 治彦 , 松田 巌 , 原田 慈久 , 放射光 **36**, 10 (2023).

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5. Propagation-based phase-contrast imaging method for full-field X-ray microscopy using advanced Kirkpatrick–Baez mirrors: Y. Tanaka, J. Yamada, T. Inoue, T. Kimura, M. Shimura, Y. Kohmura, M. Yabashi, T. Ishikawa, K. Yamauchi and S. Matsuyama, Optics Express **31(16)**, 26135-26135 (2023).

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