# Publications (2022.1 - 2023.4)

## 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 2022 are (1) to develop the doped EDOT(3,4-ethylenedioxythiophene)-based oligomer conductors, (2) to discover novel anhydrous molecular superproton conductivity of imidazolium dihydrogen phosphate, and (3) to develop ambipolar nickel dithiolene complex semiconductors.

1. Terahertz Radiation with Multi-Narrowband Components via Photoinduced Melting of Charge Order in an Electronic-Type Ferroelectric Organic α-$(BEDT\text{-}TTF)_2I_3$: Y. Kinoshita, H. Yamakawa, T. Miyamoto, K. Yamamoto, H. Mori, H. Okamoto and N. Kida, J. Phys. Soc. Jpn. 91, 094705 (2022).

2. *Charge and spin interplay in a molecular-dimer-based organic Mott insulator: N. Drichko, S. Sugiura, M. Yamashita, A. Ueda, S. Uji, N. Hassan, Y. Sunairi, H. Mori, E. I. Zhilyaeva, S. Torunova and R. N. Lyubovskaya, Phys. Rev. B 106, 064202 (2022).

3. †Proton–electron-coupled functionalities of conductivity, magnetism, and optical properties in molecular crystals: H. Mori, S. Yokomori, S. Dekura and A. Ueda, Chem. Commun. 58, 5668 (2022).

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

5. *Band-filling effects in single-crystalline oligomer models for doped PEDOT: 3,4-ethylenedioxythiophene (EDOT) dimer salt with hydrogen-bonded infinite sulfate anion chains: R. Kameyama, T. Fujino, S. Dekura, S. Imajo, T. Miyamoto, H. Okamoto and H. Mori, J. Mater. Chem. C 10, 7543 (2022).

6. †Molecular Arrangement Control of [1]Benzothieno[3,2- b ][1]benzothiophene (BTBT) via Charge-Assisted Hydrogen Bond: R. Akai, K. Oka, S. Dekura, H. Mori and N. Tohnai, BCSJ 95, 1178 (2022).

7. Isotropic Anhydrous Superprotonic Conductivity Cooperated with Installed Imidazolium Molecular Motions in a 3D Hydrogen-Bonded Phosphate Network: S. Dekura, M. Mizuno and H. Mori, Angew Chem Int Ed 61, e202212872(1-7) (2022).

8. †*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 (2023).

9. †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).

10. †*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).

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

### Osada group

We have theoretically and experimentally established that the quantum thermoelectric Hall effect (QTHE) appears even in the 3D semimetals with straight nodal lines. It corresponds to the QTHE in 3D Dirac/Weyl semimetals with nodal points. In the QTHE, the plateau-like constant thermoelectric Hall conductivity $\alpha_{xy}$ is observed at the high-magnetic-field quantum limit. When the magnetic field is parallel to the nodal lines, the n=0 ground Landau subband of the nodal line semimetal plays the similar role as the pair of the n=0 chiral Landau subbands of Dirac/Weyl semimetals. We successfully observed the QTHE, which quantitatively agrees with the theoretical calculation, in bulk graphite with straight nodal lines. We also discussed the

* Joint research among groups within ISSP.

dimensional crossover of the QTHE from 3D to 2D in graphite thin-films.

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

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

3. Weak localization on moire superlattice in twisted double bilayer graphene: M. Kashiwagi, T. Taen, K. Uchida, K. Watanabe, T. Taniguchi and T. Osada, Jpn. J. Appl. Phys. **61**, 100907(1-5) (2022).

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

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

6. 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).

## 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) ultralow-temperature resistivity measurements of $UTe_2$, (2) thermal-Hall measurements of AFM skyrmions in $MnSc_2S_4$, (3) spontaneous thermal Hall measurements of candidate materials of chiral superconductivity, and (4) NMR measurements of $EuIn_2As_2$.

1. Anomalous electromagnetic response in the spin-triplet superconductor $UTe_2$: Y. Shimizu, S. Kittaka, Y. Kono, T. Sakakibara, K. Machida, A. Nakamura, D. Li, Y. Homma, Y. J. Sato, A. Miyake, M. Yamashita and D. Aoki, Phys. Rev. B **106**, 214525 (2022).

2. [*]Charge and spin interplay in a molecular-dimer-based organic Mott insulator: N. Drichko, S. Sugiura, M. Yamashita, A. Ueda, S. Uji, N. Hassan, Y. Sunairi, H. Mori, E. I. Zhilyaeva, S. Torunova and R. N. Lyubovskaya, Phys. Rev. B **106**, 064202 (2022).

3. Resistivity and thermal conductivity of an organic insulator $\beta'$–$EtMe_3Sb[Pd(dmit)_2]_2$: M. Yamashita, Y. Sato, Y. Kasahara, S. Kasahara, T. Shibauchi and Y. Matsuda, Scientific Reports **12**, 9187 (2022).

4. Field-induced topological Hall effect in antiferromagnetic axion insulator candidate $EuIn_2As_2$: J. Yan, Z. Z. Jiang, R. C. Xiao, W. J. Lu, W. H. Song, X. B. Zhu, X. Luo, Y. P. Sun and M. Yamashita, Phys. Rev. Research **4**, 013163 (2022).

5. Planar thermal Hall effects in the Kitaev spin liquid candidate $Na_2Co_2TeO_6$: H. Takeda, J. Mai, M. Akazawa, K. Tamura, J. Yan, K. Moovendaran, K. Raju, R. Sankar, K.-Y. Choi and M. Yamashita, Phys. Rev. Research **4**, L042035 (2022).

6. Topological thermal Hall effect of magnons in magnetic skyrmion lattice: M. Akazawa, H.-Y. Lee, H. Takeda, Y. Fujima, Y. Tokunaga, T.-H. Arima, J. H. Han and M. Yamashita, Phys. Rev. Research **4**, 043085 (2022).

## Ideue group

We have investigated the optical and magnetic properties of layered van der Waals crystals. By applying strain, we have successfully controlled the symmetry of 3R-$MoS_2$ and demonstrated the giant enhancement of bulk photovoltaic effect reflecting the polar structure. In addition, we have clarified that photovoltaic property along the out-of-plane direction is affected by the stacking sequence of two-dimensional semiconductors. We have also reported the effective modulation of magnetic properties such as transition temperature and magnetic anisotropy by applying pressure or electrolyte gating.

1. 空間反転対称性の破れた結晶における整流現象 : 井手上 敏也 , 板橋 勇輝 , 岩佐 義宏 , 日本物理学会誌 **77**, 475-480 (2022).

2. Spontaneous-polarization-induced photovoltaic effect in rhombohedrally stacked $MoS_2$: D. Yang, J. Wu, B. T. Zhou, J. Liang, T. Ideue, T. Siu, K. M. Awan, K. Watanabe, T. Taniguchi, Y. Iwasa, M. Franz and Z. Ye, Nat. Photon. **16**, 469-474 (2022).

3. Magnetic Anisotropy Control with Curie Temperature above 400 K in a van der Waals Ferromagnet for Spintronic Device: Z. Li, M. Tang, J. Huang, F. Qin, L. Ao, Z. Shen, C. Zhang, P. Chen, X. Bi, C. Qiu, Z. Yu, K. Zhai, T. Ideue, L.

[†] Joint research with outside partners.

Wang, Z. Liu, Y. Tian, Y. Iwasa and H. Yuan, Advanced Materials **34**, 2201209 (2022).

4. Giant bulk piezophotovoltaic effect in 3R-$MoS_2$: 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).

5. 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).

## Division of Condensed Matter Theory

### Tsunetsugu group

We have collaborated with the visiting professor, Dr. Hiroaki Kusunose, and investigated fundamental properties of phonons in chiral crystals. The main issue is how to characterize the splitting in the phonon energy dispersion between two chiral modes with different crystal angular momentum (CAM), which is specific to the systems with chiral crystal structure. Examining necessary conditions for their dynamical matrix, we have proved that the sound velocity is identical for the two chiral modes with CAM +1 and –1, which invalidates precedent some discussions expecting its splitting. The effects of chiral structure are manifested in a linear energy splitting of the optical phonon modes and we have derived a simple formula for its linear coefficient represented in terms of parameters in the microscopic model. This is a pseudo-scalar and related to electric toroidal monopole $G_0$ of the system.

1. *Stimulated Rayleigh Scattering Enhanced by a Longitudinal Plasma Mode in a Periodically Driven Dirac Semimetal $Cd_3As_2$: Y. Murotani, N. Kanda, T. N. Ikeda, T. Matsuda, M. Goyal, J. Yoshinobu, Y. Kobayashi, S. Stemmer and R. Matsunaga, Phys. Rev. Lett. **129**, 207402 (2022).

2. Diabatic and adiabatic transitions between Floquet states imprinted in coherent exciton emission in monolayer $WSe_2$: K. Uchida, S. Kusaba, K. Nagai, T. N. Ikeda and K. Tanaka, Science Advances **8**, eabq7281 (2022).

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

4. Floquet-Landau-Zener interferometry: Usefulness of the Floquet theory in pulse-laser-driven systems: T. N. Ikeda, S. Tanaka and Y. Kayanuma, Phys. Rev. Research **4**, 033075 (2022).

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

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

### Kato group

The main research subject of Kato Lab. is transport properties in mesoscopic and spintronic devices. We studied (1) heat transport through a two-level system under continuous quantum measurement, (2) spin pumping from ferromagnetic insulators to unconventional superconductors and anisotropic Dirac systems, (3) non-adiabatic corrections in electronic transport through a quantum dot, (4) spin Hall magnetoresistance in metals coupled with two-dimensional spin systems, (5) high-harmonic generation in distorted graphens, and (6) nonequilibrium noise in the BCS-BEC crossover.

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

2. Nonadiabatic Correction and Adiabatic Criteria of Noninteracting Quantum Dot Systems: M. Hasegawa and T. Kato, J. Phys. Soc. Jpn. **91**, 074705(1-8) (2022).

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

4. Ferromagnetic resonance modulation in d-wave superconductor/ferromagnetic insulator bilayer systems: Y. Ominato, A. Yamakage, T. Kato and M. Matsuo, Phys. Rev. B **105**, 205406(1-7) (2022).

5. Heat transport through a two-level system under continuous quantum measurement: T. Yamamoto, Y. Tokura and T. Kato, Phys. Rev. B **106**, 205419 (2022).

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6. Spin pumping into anisotropic Dirac electrons: T. Funato, T. Kato and M. Matsuo, Phys. Rev. B **106**, 144418(1-10) (2022).

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

8. †*TeNeS: Tensor network solver for quantum lattice systems: Y. Motoyama, T. Okubo, K. Yoshimi, S. Morita, T. Kato and N. Kawashima, Computer Physics Communications **279**, 108437 (2022).

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

10. †*MateriApps LIVE! and MateriApps Installer: Environment for starting and scaling up materials science simulations: Y. Motoyama, K. Yoshimi, T. Kato and S. Todo, SoftwareX **20**, 101210 (2022).

11. 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 (2023).

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

13. 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).

14. 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).

15. 電子スピンにより駆動するナノモーター : 泉田 渉 , 奥山 倫 , 加藤 岳生 , 松尾 衛 , 固体物理 **57**, 547-554 (2022).

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

17. 電磁気学入門 ( 物理学レクチャーコース ): 加藤 岳生 , ( 裳華房 , 東京 , 2022).

## Division of Nanoscale Science

### Katsumoto group

We have experimentally found that an increase in the curvature of the electron orbit increases the portion of non-adiabatic transition at the orbital corner. This is used in the realization of a "half-mirror" device in which the wave function is equally distributed between two edge states. By using the recursive Green function method, the experiment was successfully reproduced. A Mach-Zehnder (MZ) interferometer consisting of such half mirrors showed high visibility of over 60%. Moreover, the coherence length of over 0.6 mm is an order of magnitude compared to MZ interferometers using ordinary edge states. This surprisingly high coherence is attributed to the closeness of the two edge states.

1. Joule heating and the thermal conductivity of a two-dimensional electron gas at cryogenic temperatures studied by modified $3\omega$ method: A. Endo, S. Katsumoto and Y. Iye, Journal of Applied Physics **132**, 104302 (2022).

2. Anisotropic Behavior of the Thermoelectric Power and the Thermal Conductivity in a Unidirectional Lateral Superlattice: A Typical Anisotropic System Exhibiting Two Distinct Nernst Coefficients: A. Endo, S. Katsumoto and Y. Iye, J. Phys. Soc. Jpn. **92**, 044705 (2023).

3. Half-Mirror for Electrons in Quantum Hall Copropagating Edge Channels in a Mach-Zehnder Interferometer: T. Shimizu, J.-I. Ohe, A. Endo, T. Nakamura and S. Katsumoto, Phys. Rev. Applied **19**, 034085 (2023).

### Otani group

This year, our research on antiferromagnetic spintronics advanced as we successfully manipulated the cluster magnetic octupole state in $M_3X$ (X=Mn or Sn) thin films and achieved complete switching of the state using epitaxial thin films through spin-orbit torque. We also explored the spin Hall effect in the Weyl ferromagnet $Co_2MnGa$ and identified that the anomalous Nernst effect could contribute up to 75% of the total measured signal. Additionally, we investigated efficient pattern recognition with neuromorphic computing by utilizing the magnetic field-induced dynamics of skyrmions. Our research extended to magnon-phonon coupling as well, where we developed a theoretical formulation for the interaction between surface acoustic waves and spin waves in ferromagnetic thin films. Furthermore, we observed intriguing behaviors in voltage signals under out-of-plane

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external magnetic fields caused by surface acoustic wave-driven ferromagnetic resonance. Our studies on molecular chirality and metallic thin films demonstrated the chirality-induced magnetoresistance due to thermally driven spin polarization. Finally, our international collaborative investigations uncovered thickness-dependent reconfigurable spin-wave dynamics in $Ni_{80}Fe_{20}$ nanostripe arrays. We also explored the role of spin-orbit coupling in ultrafast spin dynamics in nonmagnet/ferromagnet heterostructures. These findings offer valuable insights into the fundamental mechanisms of spintronics and pave the way for developing novel technologies and applications in this rapidly-evolving field.


1. Efficient orbital torque in polycrystalline ferromagnetic−metal/Ru/$Al_2O_3$ stacks: Theory and experiment: L. Liao, F. Xue, L. Han, J. Kim, R. Zhang, L. Li, J. Liu, X. Kou, C. Song, F. Pan and Y. Otani, Phys. Rev. B **105**, 104434 (2022).

2. Perspectives on spintronics with surface acoustic waves: J. Puebla, Y. Hwang, S. Maekawa and Y. Otani, Appl. Phys. Lett. **120**, 220502 (2022).

3. *Chirality-Induced Magnetoresistance Due to Thermally Driven Spin Polarization: K. Kondou, M. Shiga, S. Sakamoto, H. Inuzuka, A. Nihonyanagi, F. Araoka, M. Kobayashi, S. Miwa, D. Miyajima and Y. Otani, J. Am. Chem. Soc. **144**, 7302-7307 (2022).

4. *Perpendicular full switching of chiral antiferromagnetic order by current: T. Higo, K. Kondou, T. Nomoto, M. Shiga, S. Sakamoto, X. Chen, D. Nishio-Hamane, R. Arita, Y. Otani, S. Miwa and S. Nakatsuji, Nature **607**, 474-479 (2022).

5. Pattern recognition with neuromorphic computing using magnetic field–induced dynamics of skyrmions: T. Yokouchi, S. Sugimoto, B. Rana, S. Seki, N. Ogawa, Y. Shiomi, S. Kasai and Y. Otani, Sci. Adv. **8**, eabq5652 (2022).

6. *Determination of spin Hall angle in the Weyl ferromagnet $Co_2MnGa$ by taking into account the thermoelectric contributions: H. Isshiki, Z. Zhu, H. Mizuno, R. Uesugi, T. Higo, S. Nakatsuji and Y. Otani, Phys. Rev. Materials **6**, 084411 (2022).

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

8. Orbital angular momentum for spintronics: J. Kim and Y. Otani, Journal of Magnetism and Magnetic Materials **563**, 169974 (2022).

9. Electric field induced parametric excitation of exchange magnons in a CoFeB/MgO junction: A. Deka, B. Rana, R. Anami, K. Miura, H. Takahashi, Y. Otani and Y. Fukuma, Phys. Rev. Research **4**, 023139 (2022).

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

11. Thickness-Dependent Reconfigurable Spin-Wave Dynamics in $Ni_{80}Fe_{20}$ Nanostripe Arrays: P. K. Pal, S. Sahoo, K. Dutta, A. Barman, S. Barman and Y. Otani, Adv Materials Inter **9**, 2201333 (2022).

12. Voltage Signals Caused by Surface Acoustic Wave Driven Ferromagnetic Resonance Under Out-of-Plane External Fields: Y. Hwang, J. Puebla, K. Kondou and Y. Otani, Adv Materials Inter **9**, 2201432 (2022).

13. Giant effective Zeeman splitting in a monolayer semiconductor realized by spin-selective strong light–matter coupling: T. P. Lyons, D. J. Gillard, C. Leblanc, J. Puebla, D. D. Solnyshkov, L. Klompmaker, I. A. Akimov, C. Louca, P. Muduli, A. Genco, M. Bayer, Y. Otani, G. Malpuech and A. I. Tartakovskii, Nat. Photon. **16**, 632 (2022).

14. Role of Spin–Orbit Coupling on Ultrafast Spin Dynamics in Nonmagnet/Ferromagnet Heterostructures: S. N. Panda, B. Rana, Y. Otani and A. Barman, Adv Quantum Tech **5**, 2200016 (2022).

15. *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).

16. *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).

17. 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).


## Hasegawa group

Disorder-induced superconductor-insulator transition (SIT) in the two-dimensional (2D) systems has been a subject of extensive studies as one of the quantum phase transitions (QPT). Recent advancements in the fabrication of highly crystalline 2D system revealed the presence of anomalous metallic state and quantum Griffiths phase around QPT. The origins of such new phases are

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still under debate partly because of lack of microscopic understanding. In 2022, we performed scanning tunnelling spectroscopy (STM) on highly-crystalline Pb monoatomic-layer superconductors formed on vicinal substrates with various miscut angles to investigate these phases microscopically and to reveal how their presences are affected by the introduction of disorder. Our results revealed the presence of stable vortices in the regime of the quantum metallic state. The vortex liquid phase, which was expected in the metallic regime, was observed in a small portion of the regime only on vicinal substrates, suggesting that the metallic resistance is driven by infinitesimal current in the transport measurements. A pseudogap was also observed above the critical magnetic fields presumably due to the localization of the Cooper pairs induced by quantum fluctuation.

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

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

3. 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).

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

## Lippmaa group

We are developing a machine learning approach to the analysis of reflection high-energy electron diffraction images. The purpose is to capture in real time, during thin film growth, the phase composition of a thin film surface. A neural network is thus used to extract diffraction features from the diffraction patterns, followed by periodicity and intensity analysis to extract composition information. Besides inorganic thin films grown by pulsed laser deposition, we study organic molecular layer formation on the water surface and the formation of Langmuir-Blodgett films.

1. Mechanical Tuning of Aggregated States for Conformation Control of Cyclized Binaphthyl at the Air–Water Interface: M. Ishii, T. Mori, W. Nakanishi, J. P. Hill, H. Sakai and K. Ariga, Langmuir **38**, 6481 (2022).

2. Critical Role of Terminating Layer in Formation of 2DEG State at the $LaInO_3$/$BaSnO_3$ Interface: S. Kim, M. Lippmaa, J. Lee, H. Cho, J. Kim, B. Kim and K. Char, Adv. Mater. Interfaces **9**, 2201781 (1-7) (2022).

3. Effects of shape and solute-solvent compatibility on the efficacy of chirality transfer: Nanoshapes in nematics: A. Nemati, L. Querciagrossa, C. Callison, S. Shadpour, D. P. N. Gonçalves, T. Mori, X. Cui, R. Ai, J. Wang, C. Zannoni and T. Hegmann, Sci. Adv. **8**, eabl4385 (2022).

4. Application of machine learning to reflection high-energy electron diffraction images for automated structural phase mapping: H. Liang, V. Stanev, A. G. Kusne, Y. Tsukahara, K. Ito, R. Takahashi, M. Lippmaa and I. Takeuchi, Phys. Rev. Materials **6**, 063805 (1-9) (2022).

5. Coordination Amphiphile: Design of Planar-Coordinated Platinum Complexes for Monolayer Formation at an Air-Water Interface Based on Ligand Characteristics and Molecular Topology: J. Adachi, M. Naito, S. Sugiura, N.-T. Le, S. Nishimura, S. Huang, S. Suzuki, S. Kawamorita, N. Komiya, J. P. Hill, K. Ariga, T. Naota and T. Mori, BCSJ **95**, 889 (2022).

6. Vortex Flow-controlled Circularly Polarized Luminescence of Achiral Pt(II) Complex Aggregates Assembled at the Air-Water Interface (Small Methods 12/2022): T. Maeda, T. Mori, M. Ikeshita, S. C. Ma, G. Muller, K. Ariga and T. Naota, Small Methods **6**, 2270071 (2022).

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[†] Joint research with outside partners.

## Yoshinobu group

We conducted several research projects in the fiscal year 2022: (1) The surface chemistry of hydrogen, formic acid and $CO_2$ on Pd-Cu(111), Cu(997), Cu(977) and Pd-Cu(977) surfaces was studied by SR-PES, IRAS, HREELS and TPD. (2) The adsorption/desorption of $CH_4$ on Pt(997) was studied by TPD, IRAS, SR-XPS and van der Waals DFT. (3) The dry reforming process of $CH_4$ with $CO_2$ on Pt(997) was studied by AP-XPS at SPring-8. (4) The reaction dynamics of CO + O -> $CO_2$ on Pt(111) was studied by ab-initio molecular dynamics (AIMD) with van der Waals DFT. (5) The reaction of $MoS_2$ basal plane and the edge of $MoS_2$ in vacuum and under hydrogen pressure was studied by AP-XPS at SPring-8 and DFT calculations. (6) Hydrogenation of $CO_2$ using a hydrogen-permeable PdCu alloy membrane, and (7) The newly constructed narrow band and broad band THz pulse system has been applied to the surface chemistry on Pt(111).


1. *Stimulated Rayleigh Scattering Enhanced by a Longitudinal Plasma Mode in a Periodically Driven Dirac Semimetal $Cd_3As_2$: Y. Murotani, N. Kanda, T. N. Ikeda, T. Matsuda, M. Goyal, J. Yoshinobu, Y. Kobayashi, S. Stemmer and R. Matsunaga, Phys. Rev. Lett. **129**, 207402 (2022).

2. †Substrate-Selective Intermolecular Interaction and the Molecular Self-Assemblies: 1,3,5-Tris(4-bromophenyl)benzene Molecules on the Ag(111) and Si(111) ($\sqrt{3} \times \sqrt{3}$)-Ag Surfaces: N. Tsukahara and J. Yoshinobu, Langmuir **38**, 8881 (2022).

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* Joint research among groups within ISSP.

## Functional Materials Group

### Akiyama group

In 2022, we studied ultra-fast gain-switching in 30GHz-modulation-bandwidth 1270nm DFB-type single-mode laser diodes (LDs) with and without chirp compensation, and realized gain-switched 5.3 ps short pulses near the Fourier transform limit. We made processing twice in a year on gain-switched 1030-1060nm InGaAs LDs with revised designs and procedures, and installed them into our original 10 ps LD-seed-pulse prototype modules. We studied on heat-recovery (HERC) solar cells, in collaboration with AIST team, and found output-power equivalence of two- and four-terminal photovoltaic-thermoelectric hybrid tandems. Time-resolved resonant Raman spectroscopy on channel rhodopsin with semiconductor-laser-based light sources has been performed in collaboration with Inoue-group within ISSP, and the first collaboration journal paper on this subject was accomplished. Collaboration work and papers with Hiyama-team in Gunma University were accomplished on quantitative spectroscopy on bioluminescence quantum yield of new luciferin analogs and on photo-cleavage/photo-bleaching quantum yields of D-luciferin and coumarin-caged-luciferins.


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† Joint research with outside partners.

## Sugino group

We have developed the exchange-correlation functional of the density functional theory for solids based on machine learning. We also studied activity of the oxygen reduction reaction occurring on the defective zirconia electrode. We further studied the cuprate superconductor using an advanced exchange-correlation functional. We also did collaborating works on the many-body greens function method, a topological material, and so on.

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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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3. Phase degree of freedom and topology in multiple-Q spin textures: K. Shimizu, S. Okumura, Y. Kato and Y. Motome, Phys. Rev. B **105**, 224405 (2022).

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5. Confinement phase in carbon-nanotubes and the extended massive Schwinger model: T. Oka, J. Phys. A: Math. Theor. **55**, 504001 (2022).

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## Inoue group

In 2022, we reported the first three-dimensional structure of *Psp*R, which is a light-driven outward $H^+$ pump without the typical

* Joint research among groups within ISSP.

cytoplasmic $H^+$ donor, by X-ray crystallography. A new type of outward $H^+$ pumping rhodopsins (SacR) was found from Saccharibacteria, a lineage of candidate phyla radiation (CPR). Interestingly, SacR has a fenestration close to the head group of the retinal chromophore in the protein body. We revealed exogenous retinal is taken up into the protein body through this fenestration. Moreover, a new microbial rhodopsin class fused with a bestrophin channel, named Bestrhodopsin, was discovered from diverse algae. The ion flux through the pore in the bestrophin part is regulated by surrounding rhodopsin parts in a light-dependent manner. Interestingly, bestrhodopsin exhibits pure all-*trans*-to-11-*cis* isomerization which was not known for microbial rhodopsins but is typical among animal rhodopsins. The kinetic study of schizorhodopsin (SzR) revealed that the kinetic isotope effect of many photo intermediate-conversion processes involving retinal deprotonation and reprotonation and activation enthalpy and entropy are much lower than that of other microbial rhodopsins. The photoreaction cycle of a new channelrhodopsin, ChRmine was also reported.


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## Quantum Materials Group

### Oshikawa group

Ballistic transport can be characterized by Drude weight, which is given by Kohn formula. Recently, we have generalized the Kohn formula to all orders of the nonlinear conductivity. However, the nonlinear Drude weights obtained by the generalized Kohn formula often diverge in the thermodynamic limit. In order to clarify this remarkable behavior, we have studied ballistic transport and its characterizations in a very simple system of the one-dimensional tight-binding model with a single defect. We showed that, even in this simple model, we can observe the divergence of nonlinear Drude weights. We emphasize that these nonlinear Drude weights are obtained by the generalized Kohn formula, which corresponds to the adiabatic limit for a given system size. As a resolution, we demonstrated that, by taking the thermodynamic limit before the adiabatic limit, low-frequency contributions merge into the Drude weight, which does not diverge. The result also does not depend on the impurity strength, thus characterizes the ballistic transport in the bulk. We propose to distinguish the Drude weight obtained by taking the thermodynamic limit first as "bulk Drude weight", and the Drude weight given by the Kohn formula, which corresponds to taking the adiabatic limit first, as "Kohn Drude weight". While the potential issue of the order of limits has been sometimes discussed within the linear response, the discrepancy between the two limits is amplified in nonlinear Drude weights.

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### 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 topological 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.

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### Miwa group

We have studied the following topics this year: (1) Spin-torque control of chiral antiferromagnet $Mn_3Sn$, (2) Chirality-induced spin selectivity with no net current, and (3) x-ray magnetic circular dichroism on a magnetic interface. In topic (1), we find that current-induced full switching of octupole polarization by using strained $Mn_3Sn$ thin film (Nature **607**, 404). This is a work in collaboration with Nakatsuji and Otani groups. In topic (2), we find that chiral molecule at the interface with metal possesses thermally-driven broken time-reversal symmetry. This is a work in collaboration with Otani group (J. Am. Chem. Soc. **144**, 7302). In topic (3), we find that electron correlation is a key to understanding interfacial magnetic anisotropy at Fe/MgO interface (ACS Appl. Electron. Mater. **4**, 1794).

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## Division of Data-Integrated Materials Science

### Fukushima group

Automatic exhaustive exploration of a large material space by high-performance supercomputers is crucial for developing new functional materials. We demonstrated the efficiency of high-throughput calculations using the all-electron Korringa–Kohn–Rostoker coherent potential approximation method with the density functional theory for the large material space consisting of quaternary high-entropy alloys, which are nonstoichiometric and substitutionally disordered materials. The exhaustive

* Joint research among groups within ISSP.

calculations were performed based on the AkaiKKR program package and supercomputer Fugaku, where the numerical parameters and self-consistent convergence are automatically controlled. The large material database including the total energies, magnetization, Curie temperature, and residual resistivity was constructed by our calculations. We used frequent itemset mining to identify the characteristics of parcels in magnetization and Curie temperature space. We also identified the elements that enhance the magnetization and Curie temperature and clarified the rough dependence of the elements through regression modeling of the residual resistivity.


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## Materials Design and Characterization Laboratory

### Hiroi group

Apart from rutile, which crystallizes in the rutile-type structure characteristic of many metal dioxides, three major polymorphs of titanium dioxide ($TiO_2$) are known: anatase, brookite, and the α-lead dioxide (α-$PbO_2$)-type high-pressure form. Ti ions are commonly found in octahedra composed of six oxide ions, and their crystal structures are distinguished according to the linkage pattern of the $TiO_6$ octahedra. Inorganic structural chemistry considers that, in the rutile and α-$PbO_2$ types, Ti ions occupy half of the octahedral voids in the hexagonal close packing of oxide ions, and the $TiO_6$ octahedra in each layer are joined via edge sharing to form linear and zigzag strands, respectively. Anatase and brookite, on the other hand, exhibit more complex three-dimensional edge-sharing octahedral connections, although their origins are not fully explained. I show that these configurations can be interpreted as distinct stacking structures of layers with α-$PbO_2$-type zigzag strands. Additionally, I characterize the crystal structures of four $TiO_2$ polymorphs in detail using stacking sequence descriptions based on anion close packings and explore their relationships in terms of inorganic structural chemistry. I note that the moderate covalent nature of the Ti–O bond and the local structural instability of $d^0$ ions result in an unusual variety of polymorphs in $TiO_2$.


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† Joint research with outside partners.

tions and electronic structure calculations: H. T. Hirose, T. Terashima, D. Hirai, Y. Matsubayashi, N. Kikugawa, D. Graf, K. Sugii, S. Sugiura, Z. Hiroi and S. Uji, Phys. Rev. B **105**, 035116 (2022).

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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 2022, (1) QMC study of Bose gases [Masaki-Kato, et al., JPSJ90], (2) Study of spin liquid in frustrated spin systems [Ogino, PRB106][Ido, et al., npj QM7], (3) Effect of boundary conditions in quantum spin clusters [Eguchi et al, JPSJ91], and (4) Development of open-source applications [Okubo et al, CPC279].

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* Joint research among groups within ISSP.

## Uwatoko group

We have performed polycrystalline and single-crystal neutron diffraction experiments to determine the magnetic structure under ambient and high pressures on the $CePtSi_2$. We found incommensurate magnetic peaks with a magnetic propagation vector of (0.32,0,0.11) at ambient pressure below $T_{SDW}$ ~ 1.25 K, which originate from a spin-density-wave order with the easy axis along the c axis and an averaged ordered moment of 0.45(5)$\mu_B$. Applying pressures, the magnetic order disappears around 1.0 GPa, which is much lower than the critical pressure for the superconducting phase. The results suggest that other than magnetic fluctuations, may play a primary role in the superconducting pairing mechanism. We discovered the first ternary Mn-based superconductor $KMn_6Bi_5$ under high pressure. Bulk superconductivity emerges in the pressurized single-crystal $KMn_6Bi_5$ when its antiferromagnetic order disappears by pressure. The optimal $^{on}T_c$ reaches ~9.3 K at 14.2 GPa, and $\mu_0H_{c2}(0)$ is found to exceed the Pauli paramagnetic limit. We investigated the superconductivity of $(TMTTF)_2TaF_6$ (TMTTF: tetramethyl-tetrathia-fulvalene) by conducting resistivity measurements under high pressure up to 8 GPa. A superconducting state in $(TMTTF)_2TaF_6$ emerged after a metal-insulator transition was suppressed with increasing external pressure. We discovered a superconducting state in $5 \leq P \leq 6$ GPa from $T_c$ = 2.1 K to 2.8 K. In addition, when the pressures with maximum SC temperatures are compared between the $PF_6$ and the $TaF_6$ salts, we found that $(TMTTF)_2TaF_6$ has a 0.75 GPa on the negative pressure side in the *T-P* phase diagram of $(TMTTF)_2TaF_6$. We have performed systematic electrical resistivity and single crystal X-ray diffraction measurements of CsCl-type cubic compound CeZn under high pressure up to 9.5 GPa. Applying the pressure, the coupled magnetic and crystal structural transition becomes separated above 1.0 GPa and then the AFM order changes to ferromagnetic (FM). The FM ordering temperature decreases with further applying pressure and changes to a nonmagnetic state above ~3.0 GPa. In the nonmagnetic state, we discovered superconductivity below $T_{sc}$ ~ 1.3 K over 5.5 GPa, which survives even up to 9.5 GPa.


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## Ozaki group

As a continuous research from the FY2021, we explored novel periodic structures of multi-sized hard spheres by a random structure searching method, and identified 60 putative densest ternary sphere packings (DTSPs), where the 59 packings have been discovered by our studies for the first time. We found that some of the discovered DTSPs are well-ordered, for example, the medium spheres in the (9-7-3) structure are placed in a straight line with comprising the unit cell, and that some of DTSPs correspond to real crystals. Our study suggests that the diverse structures of DTSPs can be effectively used as structural prototypes for searching ternary, quaternary, and quinary crystal structures. Using two DTSPs, the (13-2-1) and (13-3-1) structures, among the DTSPs as structure prototypes, we exhaustively searched quaternary metal hydrides for the 73 304 candidate hydrides, and identify 23 hydrides with static and dynamic stability, including $H_{12}ScY_2La$ and $H_{12}TiNi_3Ba$. The superconducting transition temperatures $T_c$, calculated by density functional theory for superconductors, are found to be 5.7 and 6.7 K for the selected two hydrides $H_{12}ScY_2Ca$ and $H_{12}ScY_2Sr$, respectively. We expect that the 23 candidates of hydrides screened by the exhaustive search for 73304 hydrides provide a guideline to narrow down the search space for trials in the experimental synthesis of quaternary metal hydrides.

* Joint research among groups within ISSP.

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6. †*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 (2023).

## Noguchi group

We have studied (1) theoretical analysis of isotropic and anisotropic curvature-inducing proteins onto membranes, (2) reaction-diffusion waves on a deformable membrane tube,(3) conformations of ultra-long-chain fatty acids, (4) cavitation generated by a sound wave, and (5) assembly of peptide amphiphiles.

1. Hydrophobic immiscibility controls self-sorting or co-assembly of peptide amphiphiles: R. Wakabayashi, R. Imatani, M. Katsuya, Y. Higuchi, H. Noguchi, N. Kamiya and M. Goto, Chem. Commun. **58**, 585 (2022).
2. †Conformations of Three Types of Ultra-Long-Chain Fatty Acids in Multicomponent Lipid Bilayers: K. Kawaguchi, H. Nagao, H. Shindou and H. Noguchi, J. Phys. Chem. B **126**, 9316-9324 (2022).
3. Membrane shape deformation induced by curvature-inducing proteins consisting of chiral crescent binding and intrinsically disordered domains: H. Noguchi, J. Chem. Phys. **157**, 034901(1-8) (2022).
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9. Membrane domain formation induced by binding/unbinding of curvature-inducing molecules on both membrane surfaces: H. Noguchi, Soft Matter **19**, 679-688 (2023).
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12. 曲率誘導タンパク質の反応拡散による生体膜のパターン形成 : 野口 博司 , 為本 尚樹 , 生物物理 **62**, 338-340 (2022).

## Yoshimi group

We have developed and enhanced the usability of programs adopted in the project for advancement of software usability in materials science (PASUMS). Our group's activity of 2022 include functional and usability enhancement of (1) abICS and (2) H-wave. We published five papers about the developed software packages (PHYSBO, TeNeS, 2DMAT, abICS and MateriApp-

† Joint research with outside partners.

sInstaller) in PASUMS. In addition, using the software packages developed by PASUMS, we have studied electronic properties of organic conductors such as β'-[Pd(dmit)$_2$]$_2$, α-(BEDT-TTF)$_2$I$_3$ and α-(BEDT-TSeF)$_2$I$_3$.


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

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6. sim-trhepd-rheed – Open-source simulator of total-reflection high-energy positron diffraction (TRHEPD) and reflection high-energy electron diffraction (RHEED): T. Hanada, Y. Motoyama, K. Yoshimi and T. Hoshi, Computer Physics Communications **277**, 108371 (2022).

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11. *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 (2023).

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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 chromium tellurides and iridium and tungsten oxides. (1) We showed that sintered samples of Cr telluride $Cr_3Te_4$ and $Cr_2Te_3$ exhibit large magnetic-field-induced strains accompanied by large volume changes though the different mechanism from magnetostriction in ferromagnetic metals. In $Cr_3Te_4$, volume increases of 500-1170 ppm by applying a magnetic field of 9 T are observed over the entire temperature range below 350 K. (2) Physical properties of sintered samples of $Ca_2Ir_2O_7$, in which pentavalent Ir atoms with $5d^4$ electron configuration form a pyrochlore structure, have been studied. The obtained experimental data strongly suggest that $Ca_2Ir_2O_7$ is metallic below room temperature and exhibits no electronic or magnetic phase transitions above 0.12 K.


1. †Electronic Properties of Pyrochlore-Type $Ca_2Ir_2O_7$: Y. Nakayama, Y. Okamoto, D. Hirai and K. Takenaka, J. Phys. Soc. Jpn. **91**, 125002(1-2) (2022).

2. Electronic structure reconstruction by trimer formation in $CsW_2O_6$ studied by x-ray photoelectron spectroscopy: R. Nakamura, D. Takegami, A. Melendez-Sans, L. H. Tjeng, M. Okawa, T. Miyoshino, N. L. Saini, M. Kitamura, D. Shiga, H. Kumigashira, M. Yoshimura, K. -D. Tsuei, Y. Okamoto and T. Mizokawa, Phys. Rev. B **106**, 195104(1-6) (2022).


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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).

## 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 2022, we obtained great progress for structural studies on molecular liquids under high pressure. We have performed synchrotron-radiation X-ray diffraction works using a Paris-Edinburgh cell (< 5 GPa) and BL37XU, where focusing high energy X-ray is available, at SPring-8. A new anvil system workable at low temperature (200-300 K) was developed for our experiments. Neutron diffraction experiments were also conducted using the high-pressure instrument BL11, PLANET at J-PARC. The target materials are toluene, which is a typical van der Walls liquid and a series of polyalcohols, methanol $CH_3OH$, ethylene glycol $CH_2(OH)CH_2(OH)$, and glycerol $CH_2(OH)CH(OH)CH_2(OH)$. For toluene, we found that the intermolecular correlation is developed under high pressure, and that orientationally ordered structure is not changed much at low temperature. For glycerol and ethylene glycol, more compact intramolecular structures keeping hydrogen bonds were found under high pressure and their structures were not changed much at low temperature. Methanol exhibited intermediate pressure and temperature change between toluene and glycerol (and ethylene glycol). These results are partly confirmed by classical and the ab initio (Car-Parinello) MD simulations. The present results are completely new and will give a great impact on future research of glass transitions. Other than these results, we have obtained many interesting heat capacity and quasielastic neutron scattering (QENS) data on MOF (metal-organic-framework) and clathrate hydrate systems using our custom-made adiabatic calorimeters and the C3-1-1, AGNES spectrometer that we are managing at JRR-3, JAEA.

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2. Synergistic Stimulation of Metal-Organic Frameworks for Stable Super-cooled Liquid and Quenched Glass: Z. Yin, Y. Zhao, S. Wan, J. Yang, Z. Shi, S. -X. Peng, M. -Z. Chen, T. -Y. Xie, T. -W. Zeng, O. Yamamuro, M. Nirei, H. Akiba, Y. -B. Zhang, H. -B. Yu and M. -H. Zeng, J. Am. Chem. Soc. **144**, 13021-13025 (2022).

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8. The phase diagram of the API benzocaine and its highly persistent, metastable crystalline polymorphs: I. B. Rietveld, H. Akiba, O. Yamamuro, M. D. Barrio, R. Céolin and J. L. Tamarit, Pharmaceutics **15**, in press (2023).

### 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; magnetic diffuse and quasi-elastic scatterings in frustrated magnet $YBaCo_4O_7$, anomalous magnetic moment direction under magnetic anisotropy originated from crystalline electric field in van der Waals compounds

[†] Joint research with outside partners.

$CeTe_3$ and $CeTe_2Se$, damped dirac magnon in the metallic kagome antiferromagnet FeSn.


1. Anomalous Magnetic Moment Direction under Magnetic Anisotropy Originated from Crystalline Electric Field in van der Waals Compounds $CeTe_3$ and $CeTe_2Se$: D. Ueta, R. Kobayashi, H. Sawada, Y. Iwata, S.-I. Yano, S. Kuniyoshi, Y. Fujisawa, T. Masuda, Y. Okada and S. Itoh, J. Phys. Soc. Jpn. **91**, 094706(1-6) (2022).

2. Magnetic Diffuse and Quasi-Elastic Scatterings in Frustrated Magnet $YBaCo_4O_7$: M. Soda, M. Kofu, S. Ohira-Kawamura, S. Asai, T. Masuda, H. Yoshizawa and H. Kawano-Furukawa, J. Phys. Soc. Jpn. **91**, 094707(1-5) (2022).

3. Damped Dirac magnon in the metallic kagome antiferromagnet FeSn: S.-H. Do, K. Kaneko, R. Kajimoto, K. Kamazawa, M. B. Stone, J. Y. Y. Lin, S. Itoh, T. Masuda, G. D. Samolyuk, E. Dagotto, W. R. Meier, B. C. Sales, H. Miao and A. D. Christianson, Phys. Rev. B **105**, L180403(1-6) (2022).

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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 research collaborations is the magnetic structure analysis of the van der Waals magnet $CoTa_3S_6$. Prof. Seki's group in the University of Tokyo synthesized single crystals of this compound, and found that this compound exhibits a large spontaneous Hall effect without accompanying ferromagnetic moment. Temperature variations of the Hall resistivity and magnetic susceptibility indicate that the large Hall effect is induced by an antiferromagnetic order at low temperatures. We performed polarized neutron scattering experiment at PONTA, revealing that the spontaneous Hall effect arises from an all-in-all-out type non-coplanar magnetic order with broken time-reversal symmetry, which can be a source of the Hall effect.


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

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

3. †Polarized neutron scattering study of the centrosymmetric skyrmion host material $Gd_2PdSi_3$: J. Ju, H. Saito, T. Kurumaji, M. Hirschberger, A. Kikkawa, Y. Taguchi, T.-H. Arima, Y. Tokura and T. Nakajima, Phys. Rev. B 107, 024405 (2023).

4. †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. Khanh, K. Karube, H. Saito, D. Hashizume, R. Kiyanagi, Y. Tokura, R. Arita, T. Nakajima and S. Seki, Nat. Phys., (advanced online publication) (2023).

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## Mayumi group

Mayumi group has found that strain-induced crystallization occurs in simple polymer gels with homogeneous network structures. Also, we have performed quasi-elastic neutron scattering experiments on stretched polymer gels to detect the local strain distribution in the deformed polymer networks.


1. Quasi-elastic neutron scattering study on dynamics of polymer gels with controlled inhomogeneity under uniaxial deformation: K. Aomura, Y. Yasuda, T. Yamada, T. Sakai and K. Mayumi, Soft Matter **19**, 147-152 (2022).

2. †High-yield one-pot synthesis of polyrotaxanes with tunable well-defined threading ratios over a wide range: T. Noritomi, L. Jiang, H. Yokoyama, K. Mayumi and K. Ito, RSC Advances **12**, 3796–3800 (2022).

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


* Joint research among groups within ISSP.

4. A neuromechanical model for Drosophila larval crawling based on physical measurements: X. Sun, Y. Liu, C. Liu, K. Mayumi, K. Ito, A. Nose and H. Kohsaka, BMC Biol **20**, 130 (2022).

5. Fabrication of Polyelectrolyte Sheets of Unimolecular Thickness via MOF-Templated Polymerization: A. Nishijima, Y. Hayashi, K. Mayumi, N. Hosono and T. Uemura, Macromolecules **56**, 3141–3148 (2023).

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## International MegaGauss Science Laboratory

### Kindo group

We have installed a super-capacitor bank for long pulsed magnet. The bank has a capability of generating magnetic field of 60 T with a duration of 1 to 2 seconds. The bank consists of three units. Each unit has the maximum energy of 60 MJ, 60 MJ and 30 MJ. The maximum current is 18 kA, 18 kA and 9 kA, respectively.

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## Tokunaga group

We newly developed a long-distance optical microscope that can be installed in PPMS. We successfully obtained surface morphology in a magnetic shape-memory alloy using this system. In addition to this, we used various techniques, *e.g.*, magnetization, magnetoresistance, dielectric constant, and magnetostriction, to study various magnetic materials, topological semimetals, superconductors, and semiconductors.

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## Y. Matsuda group

Ultrahigh magnetic field research in the range of 500 T has been developing and the insulator-metal phase transition induced by such high magnetic fields is observed in $VO_2$ as well as in $SmB_6$. As for $VO_2$, the review article was published along with details of technical developments on the electromagnetic flux compression 1000 T field generator. Breathing pyrochlore compound possesses strong spin-lattice coupling and exhibits a variety of quantum phases in high magnetic fields; $CuInCr_4S_8$ has been studied with multi probes such as magnetization, striction, and dielectric constant. Several intriguing magnetic systems, a poler magnet $CaBaCo_4O_7$, a dimer magnet $Ni_2V_2O_7$, and a triangle lattice magnet $Ca_3ReO_5Cl_2$ have also studied in high magnetic fields. The review of the high magnetic field phases in solid and liquid oxygen has also been reported. The potential field-induced liquid-liquid phase transition is still uncovered and required to do continuous research. As new technical progress, a portable single-turn coil system termed PINK-01 was developed and applied to the X-ray free electron laser experiment. The X-ray diffraction up to 77 T has been performed and a structural transformation in a Mn-oxide was observed.

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We have investigated various high-field properties. In magnetic materials, such as $CuInCr_4S_8$, $Ca_3ReO_5Cl_2$, $HaCr_2O_4$, BIP-TENO, and $SrCu_2(BO_3)_2$, the field induced phase transitions have been investigated by magnetization and calorimetry in non-destructive and destructive magnetic fields. In two dimensional conductors, $SrRuO_3$, alpha$(BETS)_2I_3$, and $SrAs_3$, we have investigated the topological properties. Here, the TDO and resistivity measurements have revealed rich transport phenomena in two dimensional materials. Using newly developed rf technique, we have determined the critical field of SmFeAsO at the low temperature limit. We have also succeeded to measure the thermal conductivity for the first time in pulsed magnet.

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## Laser and Synchrotron Research Center

### Kobayashi group

We are studing a combination between an artificial intelligence and a laser material processing, aiming a construction of a theory.

1. *Stimulated Rayleigh Scattering Enhanced by a Longitudinal Plasma Mode in a Periodically Driven Dirac Semimetal $Cd_3As_2$: Y. Murotani, N. Kanda, T. N. Ikeda, T. Matsuda, M. Goyal, J. Yoshinobu, Y. Kobayashi, S. Stemmer and R. Matsunaga, Phys. Rev. Lett. **129**, 207402 (2022).

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### Harada group

Application of soft X-ray emission spectroscopy has been significantly advanced, and research on the behavior of interfacial water on the surface of diverse polymer materials have been realized by developing the precise humidification system. As a representative example of this application hydrogen-bonded structure of water on the surface of PMEA, a material used for blood tubing in ECMO against COVID-19, was clarified by comparing infrared spectroscopy and DFT calculations, and a comparison of X-ray emission spectroscopy with AFM revealed that water molecules induce phase separation of polymers and change their biocompatibility. After more than a decade of debate, a theory explaining both the temperature and isotope dependence of soft X-ray emission spectra was completed, and the X-ray emission results of liquid water published since 2008 were finally validated. The electronic state changes of transition metals during charging and discharging of the cathode material $LiMn_2O_4$ and the anode material $Fe_2O_3$ of lithium-ion batteries were clarified using operando spectroscopy. The CREST project, which aims to integrate soft and hard X-ray imaging techniques with information science, has started, and we reported on high-resolution soft X-ray imaging using a Walter mirror in collaboration with Prof. Kimura's group.

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## I. Matsuda group

We have devoted ourselves to a project of developing the next-generation synchrotron radiation (SR) facility, NanoTerasu, at Sendai in Miyagi-prefecture. To focus on the project, we discontinued the joint-research at the beamline, SPring-8 BL07LSU, in August. Subsequently, we packed our instruments, two undulators, ambient-pressure XPS system and process-informatics robot units. Then, we successfully transferred them to the NanoTerasu beamlines by the end of the fiscal year. At the X-ray free electron laser (XFEL) beamline, SACLA BL-1, we have developed a new method of nonlinear X-ray spectroscopy and achieved fruitful science of the functional materials. Based on the SR and XFEL experiments, we have also succeeded in synthesizing boron nanomaterials and in unveiling their intriguing physical/chemical properties.

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## Itatani group

By using soft X-ray attosecond pulses, we have performed soft X-ray transient absorption spectroscopy of ring-opening reaction dynamics associated with photo-absorption of a ring-shaped molecule 1,3-cyclohexadiene. We found that the Woodward-Hoffmann rule for molecular orbital symmetry holds even in transient chemical reaction states for the first time. Development of a new soft X-ray beamline with a flat water jet was initiated to expand the variation of samples from gas phase to condensed matters. High harmonic generation in the flat water jet was also examined with intense MIR pulses, and we obtained a unique vibrational signal due to molecular vibration. Photoelectron re-scattering experiments associated with tunnel ionization were performed using carrier-envelope phase (CEP)-stable intense ultrashort pulses in the infrared region. The CEP dependence of the momentum distribution of photoelectrons due to backward re-scattering was measured for Kr atoms and $CO_2$ molecules with nearly equal ionization potentials, and the differential scattering cross sections were derived. We also successfully extracted the influence of the multi-center scattering effect in the case of $CO_2$ molecules. As for the light source R&D, we have developed a highly CEP-stable infrared light source in the 2 μm region, which is excited by a Yb solid-state laser operating at 100 kHz repetition rate.

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## Kondo group

We found evidence for the multipole polaron state in the devil's staircase of CeSb, and presented selective observation of surface and bulk bands in polar $WTe_2$. We also revealed band structure leading to a large anomalous Hall effect in the noncentrosymmetric antiferromagnet $CoNb_3S_6$.

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6. *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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## Matsunaga group

We have studied light-matter interactions and light-induced nonequilibrium phenomena in solids by utilizing terahertz (THz) pulse. By using a phase-stable broadband multiterahertz pulses (10-45 THz, 40-180 meV, or 7-30 μm) with the pulse width of

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28 fs, we investigated dynamics of broadband response functions of a 3D Dirac semimetal $Cd_3As_2$ under intense periodic light wave with 30 THz frequency. We found a sharp increase of absorption at 28 THz and negative conductivity with optical gain at 31 THz. The drastic change of the spectrum can be explained by the stimulated Rayleigh scattering, which is remarkably enhanced at the frequency close to the longitudinal plasma resonance. The results suggest potential application for nondissipative slow light generation using conducting material at room temperature.


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## Okazaki group

We have investigated the superconducting-gap structures of unconventional superconductors by using a low-temperature and high-resolution laser ARPES apparatus and transient electronic structures in photo-excited non-equilibrium states by using a time-resolved ARPES apparatus using EUV and SX lasers. In the academic year 2022, we have revealed the superconducting gap structures of $CsV_3Sb_5$-derived Kagome superconductors by high-resolution laser ARPES. In addition, we have developed a tunable mid-infrared pump system for HHG laser time-resolved ARPES.


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† Joint research with outside partners.

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## Kimura group

In FY2022, the Kimura Lab. worked on the development of soft X-ray nanoimaging techniques using SPring-8 and SACLA. In experiments on SPring-8 BL07LSU, we developed a soft X-ray ptychography system using a total-reflection Wolter mirror to achieve absorption and phase imaging with a resolution of 50 nm, and succeeded in multi-wavelength imaging using mammalian cells. We also attempted to demonstrate femtosecond single-shot femtosecond spectromicroscopy imaging using a multi-aperture grating in experiments at SACLA BL1. Using a transmission type grating fabricated by electron beam lithography and a total reflection Walter mirror, we succeeded in single pulse measurement of the two-dimensional spectral distribution of an X-ray free electron laser emitted by self-amplified spontaneous emission.

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* Joint research among groups within ISSP.