

3.4 Cooperative Phenomena in Complex Macroscopic Systems

Molecular Simulation Contributions to Biological Membrane and Energy Materials Research

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During the last fiscal year, the supercomputing resources allocated to this project supported major advances in the molecular understanding of biological membranes, biomolecular interfaces, and energy materials. By combining coarse-grained and all-atom molecular dynamics simulations with free-energy calculations and enhanced sampling, we published twelve peer-reviewed papers. These results demonstrate the value of large-scale molecular simulation in connecting molecular structure and dynamics with experimentally observed properties and functions.

A central achievement was the development and application of the SPICA coarse-grained force field to complex membrane-related systems. In [1] and [2], we developed nucleic-acid and ionizable lipid nanoparticle models and used them to study lipoplexes and lipid nanoparticles relevant to nucleic acid delivery. These studies reproduced experimentally observed structural features and provided molecular insight into lipid-dependent delivery performance. In [3], simulations clarified the mechanism of transient multilamellar structure formation during ethanol-induced vesicle

transformation. In [4], simulation-guided analysis supported the design of a melittin-derived peptide with improved cytosolic delivery efficiency. In [5], we reported the first coarse-grained simulation of the hepatitis B virus envelope–capsid complex, revealing key capsid–envelope interactions and reduced lipid mobility in the viral envelope. In [6], simulations of asymmetric plasma membranes showed marked leaflet-dependent organization, with dynamic nanoscale domains emerging mainly in the inner leaflet.

The project also advanced the study of biomolecular interfaces and membrane proteins. In [7], we extended the SPICA force field to polymeric biomaterial surfaces and showed that surface hydrophobicity is a major factor governing protein adsorption, providing guidelines for the design of biocompatible polymers. In [8], molecular dynamics simulations, together with structural and functional studies, clarified the citrate transport mechanism of the barley membrane transporter HvAACT1, which is important for aluminum tolerance in crops. In [9], we applied the enhanced path-sampling method ∞ RETIS to

membrane pore formation and identified the sequence of thinning, defect formation, and pore development.

In parallel, the project produced significant results in electrolyte science for next-generation batteries. In [10], we summarized electrolyte design principles based on ion dynamics and Onsager transport coefficients. In [11], we showed that heterogeneous speciation in lithium electrolytes strongly affects experimentally observed transport properties and can cause discrepancies in lithium transference numbers. In [12], we reported polymer-assisted supercooled lithium salts as a new class of nonflammable single-ion conducting liquid electrolytes with near-unity lithium transference number and promising battery performance.

Overall, the twelve papers published during the reporting period highlight the wide scope of this project, covering force-field development, membrane remodeling, viral and peptide–membrane systems, membrane proteins, biomaterial interfaces, and battery electrolytes. Supercomputing resources were essential for simulating large and complex systems, sampling slow or rare processes, and obtaining quantitative molecular insight. These achievements have strengthened the foundation for both biological membrane research and energy materials design.

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Multiscale Molecular Dynamics Analysis of Cavitation and Chemical Reactions at Sliding Interfaces

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Achieving low friction and high durability in mechanical systems is a critical challenge for a sustainable society, as approximately 23% of global energy consumption is lost to friction [1]. Especially in resource-limited societies, advancing energy and resource conservation through the control of friction and wear is a paramount task. While water lubrication is a key technology, its ultra-low viscosity and limited load-capacity cause inadequate lubrication and cavitation significantly impacts safety and performance; thus, controlling cavitation is essential for the efficient operation of mechanical systems. In this study, we investigate interfacial phenomena across multiple length scales by combining large-scale coarse-grained molecular dynamics (CGMD) simulations and reactive molecular dynamics (RMD) simulations.

First, CGMD simulations were employed to examine whether nanoindentation at experimental scales can be realized. The coarse-grained method described in Ref. [2] was adopted. Simulations with up to several hundred million coarse-grained particles were performed, and indentation responses were

successfully obtained using an indenter geometry identical to that used in experiments.

Based on the mechanical and environmental conditions obtained from the CGMD, reactive molecular dynamics simulations were further extended to describe local chemical reactions. To this end, boundary conditions allowing material inflow and outflow were introduced, enabling a pseudo-open system, and the feasibility of maintaining a quasi-steady-state environment was examined. As a representative and well-studied system for water lubrication, hydrogen-terminated diamond-like carbon (DLC) interfaces were selected as a test case. This system has been extensively investigated in previous studies, making it suitable for assessing the validity and limitations of the proposed RMD simulation. This analysis serves as a fundamental validation to reconstruct the localized high-temperature and high-pressure environments typically observed during cavitation bubble collapse.

Observations of hydrogen-terminated DLC surfaces indicated that a quasi-steady atmosphere could be maintained only during the initial stages of sliding. As wear progressed,

a clogging state developed at the fluid interface, which obstructed material inflow and prevented sustained steady-state conditions. In addition, the employed reactive force field led to excessive H_3O^+ generation, indicating that the combined treatment of charge neutrality and molecular insertion/deletion can induce nonphysical reactions in the pseudo-open RMD simulation.

These results clarify that the simultaneous treatment of charge neutrality and molecular insertion/deletion poses a significant challenge in the current RMD simulation. Identifying these factors is a crucial step toward refining the algorithm to suppress such nonphysical reactions. Future work will focus on redesigning boundary conditions to prevent interface clogging and re-optimizing the reactive force field parameters to achieve a sustained quasi-steady state and more accurate reaction analysis.

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String Breaking and Multi-Spinon Complexes near Deconfined Quantum Criticality

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In the valence-bond solid (VBS) phase of a two-dimensional quantum magnet, spinons are elementary topological excitations realized as the nexus of four domain walls. The geometry of the square lattice enforces a parity constraint that neighboring spinons must be located in the opposite sublattice, which can be viewed as analogous to a charge constraint in particle physics. This sublattice constraint was argued to play a role at the Néel-VBS quantum phase transition [1] that is suspected to be generically a *deconfined quantum critical point* (DQCP). In the argument, the spinons form a network interconnected by domain walls giving rise to an effective AFM interaction among the spinons in a two-dimensional geometry, thereby connecting the two seemingly unrelated phases nontrivially. While hadron bound states like protons are the central objects in quantum chromodynamics and their multi-quark extensions (e.g. pentaquarks etc) and their properties are being actively studied, analogous multi-spinon bound states in condensed matter systems, especially under similarly nontrivial geometric and topological constraints, remain much more elusive.

In this work, we study a square-lattice VBS ground state with large-scale quantum Monte Carlo (QMC) simulation to see what type of multi-spinon complexes are stable and explore the constraints they accompany other than the previously argued sublattice constraint. The Hamiltonian is defined to be

$$H = -Q \sum P_{ij} P_{kl}, \quad (1)$$

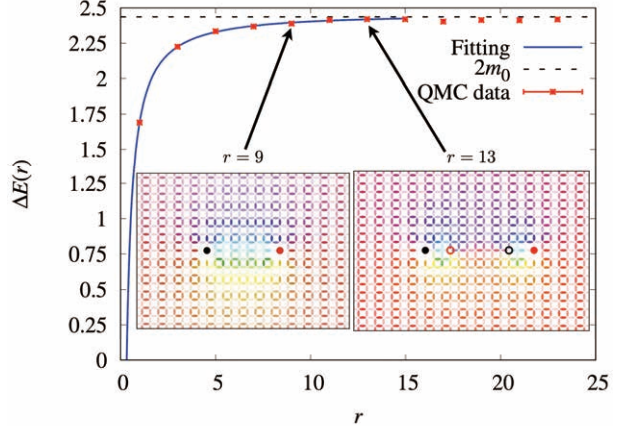


Figure 1: Excitation energy $\Delta E(r)$ as a function of the distance r between the two injected spinons. Two exemplifying configurations are shown for $r = 9$ (spinon dipole) and $r = 13$ (string breaking with emergent spinons).

where $P_{ij} = 1/4 - \mathbf{S}_i \cdot \mathbf{S}_j$ is the singlet projector, and the summation is taken over all parallel pair of bonds (i, j) and (k, l) in a plaquette of the $L \times L$ square lattice with periodic boundary condition. We set the unit $Q = k_B = 1$ and inverse temperature $\beta = L$ to effectively observe the ground state. Note that the Hamiltonian above is in the VBS phase but with a nearby proximate DQCP of the so-called JQ model [2]. We inject spinons by adding infinitely strong magnetic fields $\pm h S_i^z$ with $h \rightarrow \infty$ to a specific spin i in the system.

As a first step, we can observe two-spinon bound states forming a “dipole” with four domain walls connecting them (Fig. 1). Upon in-

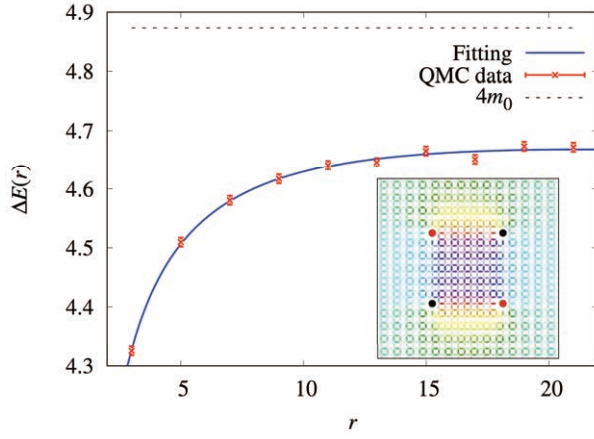


Figure 2: Excitation energy $\Delta E(r)$ as a function of the distance r between the four injected spinons in a square shape. Inset shows an exemplifying configuration.

creasing the distance between the two spinons, the strings break by spontaneously creating two emergent spinons that pair up with the two enforced spinons. This phenomenon is known as string breaking and has been studied in the context of gauge theories realizable with cold atom systems [3]. We can directly observe this using QMC, by visualizing the thermal average of the singlet density $\langle P_{ij} \rangle$ and associating a local two-dimensional VBS order parameter.

Equipped by the two-spinon bound state, we can proceed to create excitations that involve a larger number of spinons. For example, a four-spinon structure as in Fig. 2 can be seen to be far more stable than the two-spinon bound state, since the excitation energy only converges to the $r \rightarrow \infty$ limit very slowly. This means that the string breaking only happens at a far larger distance compared to the spinon dipole case.

We further found that the stable pattern with four spinons can form a network of spinons that extends to the system-size as shown in Fig. 3(a). These networks are stable against perturbations, and does not need to be periodic as can be seen from (b) with tilted angles for the four injected spinons and (c)

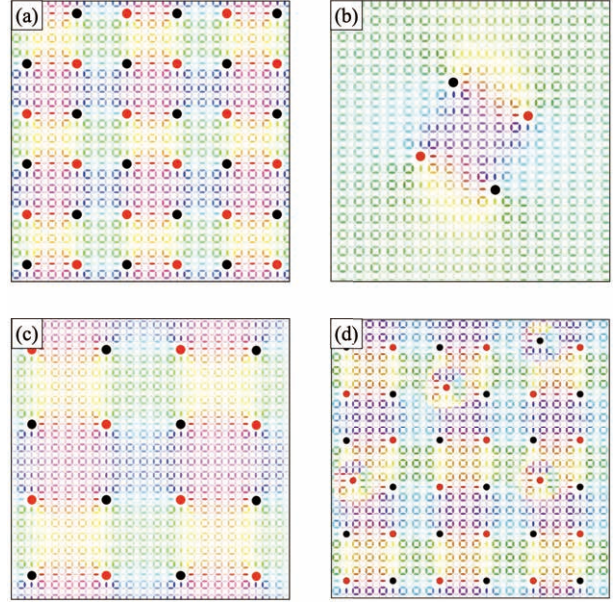


Figure 3: Several QMC configurations showing a domain-wall network.

with larger distance between the spinons. On the other hand, moving the injected spinons by (1,1) lattice spacing destroys the clean domain wall network as shown in (d), although it conserves the sublattice. We find that a *sub*-sublattice structure of the square lattice leads to this destruction because this (1,1) shift adds a π phase in the local VBS ordering. This additional constraint seems to be never addressed before in the field theory of VBS states, and raises questions about what additional considerations are needed to understand the DQCP and its relation to topological excitations.

This work was done in collaboration with Zhiyao Ning, Xuefeng Zhang, and Naoki Kawashima.

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Thermal Hall transport in frustrated magnets

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Frustrated magnets are known to host exotic quantum states, such as quantum spin liquids and complex spin textures. In recent years, thermal Hall transport has attracted considerable attention as a powerful experimental probe of such unconventional magnetic states. In particular, the observation of a half-quantized thermal Hall conductivity in the Kitaev candidate material α - RuCl_3 under magnetic fields has stimulated extensive theoretical and experimental studies [1, 2]. Understanding the microscopic origin and finite-temperature behavior of thermal Hall transport in frustrated magnets has therefore become an important issue in condensed matter physics.

In this project, we developed numerical approaches based on finite-temperature tensor network methods to investigate thermal Hall transport phenomena in frustrated quantum magnets. Since thermal Hall transport is intrinsically a finite-temperature dynamical response, reliable numerical calculations require accurate evaluations of finite-temperature equilibrium states in strongly correlated quantum systems. To address this challenge, we employed tensor network simulations based on the exponential tensor renormalization group (XTRG) method [3]. The XTRG method approximates a finite-temperature density matrix as a matrix product operator and optimizes it through imaginary time evolution, allowing us to access finite temperature properties.

First, we investigated the $S = 1/2$ Kitaev model under magnetic fields [4]. We computed finite-temperature density matrices using the

XTRG method and evaluated the temperature dependence of the thermal Hall conductivity from equilibrium spin correlations. Our results demonstrated that the thermal Hall conductivity exhibits a characteristic overshoot behavior at finite temperatures, where its value exceeds the half-quantized value expected in the zero-temperature limit. This behavior is qualitatively similar to experimental observations in α - RuCl_3 , suggesting that a simple Kitaev interaction combined with finite-temperature effects can explain the observed thermal Hall effects. We also clarified the dependence of the thermal Hall response on the direction of the applied magnetic field. In particular, the thermal Hall conductivity vanishes for magnetic fields applied parallel to the b -axis, while its sign is reversed between the a -axis and c -axis field directions. These results provide useful information for understanding the origin of anisotropic thermal transport in Kitaev materials.

In addition, we continued our investigation of the kagome-lattice Heisenberg model under magnetic fields using similar finite-temperature tensor network techniques. By systematically analyzing the magnetic-field and temperature dependence of the thermal Hall conductivity, we found that the sign reversal of the thermal Hall conductivity near the $1/9$ magnetization plateau is closely related to the stepwise development of magnetic ordering at finite temperatures [5]. This result suggests a close connection between thermal transport properties and emergent magnetic textures in frustrated systems.

The present study demonstrates that finite-temperature tensor network methods combined with large-scale supercomputing resources provide a powerful framework for investigating thermal transport phenomena in strongly correlated quantum magnets. The developed numerical techniques are expected to be applicable to a broad class of frustrated magnetic systems and to contribute to the microscopic understanding of experimentally observed thermal Hall effects.

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Thermal effects on quantum frustrated magnets

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The properties of quantum frustrated magnets at finite temperatures remain largely unexplored, and there has been a continuous demand for advancements in research based on large-scale numerical calculations. In recent years, with developments in the field of quantum information, experimentally accessible measures of quantum entanglement have attracted considerable attention. In this research project, we focused on the quantum Fisher information (QFI), which can be evaluated from dynamical spin correlations and is closely related to experimentally measurable quantities such as the dynamical spin structure factor.

As a representative example, we studied the $S = 1/2$ J_1 - J_2 triangular-lattice Heisenberg antiferromagnet. To evaluate the QFI at finite temperatures, we developed an unbiased numerical code based on the thermal pure quantum state method to calculate the dynamical spin structure factor [1, 2]. We also accelerated our computational code using MPI parallelization techniques. In particular, we were able to evaluate the temperature dependence of the QFI and the finite-temperature dynamical spin structure factor through large-scale parallel computing using the F144cpu partitions.

In this fiscal year, we investigated the quantum critical behavior reported in triangular-lattice magnetic materials such as KYbSe₂, YbZnGaO₄, and YbZn₂GaO₅. To obtain a deeper understanding of the universal nature of this quantum criticality, we studied the finite-temperature spin dynamics and the tem-

perature dependence of the QFI in the $S = 1/2$ J_1 - J_2 triangular-lattice Heisenberg model. For this purpose, we treated clusters with up to $N = 30$ sites. In particular, we calculated the temperature dependence of the QFI density near the quantum critical point between the Néel and QSL phases in the $S = 1/2$ J_1 - J_2 triangular-lattice Heisenberg model. We found that the experimentally extracted temperature dependence of the QFI for three triangular-lattice materials, KYbSe₂, YbZnGaO₄, and YbZn₂GaO₅, follows the theoretical temperature dependence of the QFI density obtained from our numerical calculations. These results indicate that the temperature dependence of the QFI provides a useful and experimentally relevant probe of universal quantum critical behavior in triangular-lattice quantum magnets.

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Symmetry-based nonlinear fluctuating hydrodynamics in one dimension

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Recently, hydrodynamic theory has emerged as a unifying framework for understanding a broad range of transport phenomena in solids, encompassing both electronic and thermal conduction. In one-dimensional systems, the conventional nonlinear fluctuating hydrodynamics (NFH) proposed as an effective theory for non-integrable many-particle systems was known to exhibit certain theoretical inconsistencies, such as requiring unphysical parameter values. In our recent work, we reconstructed the NFH equations, relying on symmetries and conservation laws without depending on microscopic Hamiltonian details [1]. Furthermore, a dynamic renormalization group (RG) analysis of this model suggested that both the sound and heat modes belong to the Kardar-Parisi-Zhang (KPZ) universality class, characterized by a dynamical exponent $z = 3/2$. In this report, we detail the methodology and results of direct numerical simulations performed on the newly formulated NFH equations to explicitly verify these theoretical predictions.

In our numerical simulations, we solve the NFH equations in the long-wavelength limit, where they are decomposed into three independent normal modes. The fundamental equation is given by:

$$(\partial_t + \alpha c_s \partial_x - D_\alpha \partial_x^2) \phi^\alpha + \sum_{\beta, \gamma} G_{\beta\gamma}^\alpha \partial_x (\phi^\beta \phi^\gamma) = \zeta^\alpha \quad (1)$$

Here, ϕ^α represents each normal mode, with the index $\alpha \in \{+, 0, -\}$ corresponding to the

right-moving sound mode, the heat mode, and the left-moving sound mode, respectively. The parameter c_s is the sound velocity, and D_α is the diffusion constant for each mode. Due to symmetry requirements, the diffusion constants of the sound modes satisfy $D_+ = D_- = D_s$. The nonlinear coupling coefficients, $G_{\beta\gamma}^\alpha$, form a parameter matrix determined by symmetry constraints such as thermal equilibrium conditions. The term ζ^α on the right-hand side represents Gaussian white noise satisfying the fluctuation-dissipation relation, with the following spatiotemporal correlation:

$$\begin{aligned} \langle \zeta^\alpha(x, t) \zeta^\beta(x', t') \rangle \\ = -2D_\alpha \delta_{\alpha\beta} \partial_x^2 \delta(t - t') \delta(x - x') \end{aligned} \quad (2)$$

To numerically solve the NFH equations, we adopted a high-precision scheme designed to strictly satisfy conservation laws at the discrete level [1]. For spatial discretization, we utilized a staggered-grid method [2]. By defining the scalar fields at the cell centers and their corresponding fluxes at the cell boundaries, the scheme naturally ensures the conservation of quantities. For time evolution, we employed a third-order stochastic Runge-Kutta (RK3) scheme [3], which provides high accuracy for integrating stochastic terms.

Based on large-scale numerical calculations, we evaluated the spatiotemporal correlation function $\mathbb{S}^\alpha(x, t) = \langle \phi^\alpha(x, t) \phi^\alpha(0, 0) \rangle$ and tested the dynamic scaling hypothesis:

$$\mathbb{S}^\alpha(x, t) = t^{-1/z} f_\alpha \left(\frac{x - \alpha c_s t}{t^{1/z}} \right) - C_\alpha, \quad (3)$$

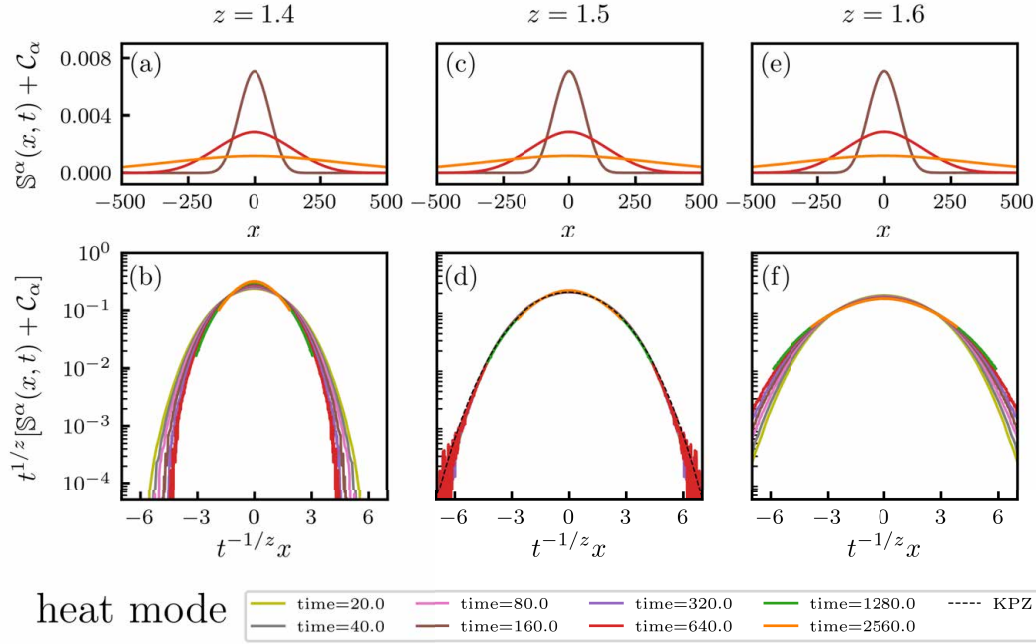


Figure 1: Dynamic scaling analysis of the spatiotemporal correlation function for the heat mode ($\alpha = 0$). Top panel: Raw data of the correlation function $\mathbb{S}^0(x, t)$ at various times. Bottom panel: Data collapse using $z = 3/2$. The horizontal axis is the scaling variable $xt^{-1/z}$ and the vertical axis is the scaled correlation function $t^{1/z}\mathbb{S}^0(x, t)$.

where $\mathcal{C}_\alpha$ is a constant offset accounting for finite-size effects.

Figure 1 shows the results specifically for the heat mode ($\alpha = 0$). By adopting $z = 1.5$, the numerical data for $\mathbb{S}^0(x, t)$ obtained at different times collapse onto a single universal curve. This excellent data collapse confirms that the dynamic scaling exponent is indeed $z = 3/2$. Furthermore, the collapsed scaling function is extremely close to the Prähofer-Spohn function, which is known as the exact scaling function of the KPZ equation.

We verified this result under various parameter settings, revealing that these findings hold robustly across different parameter changes. This demonstrates that the NFH equations, reconstructed solely from symmetry and conservation laws independent of microscopic details, accurately describe the universal KPZ scaling.

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Molecular Dynamics Study of Rayleigh-Plateau Instability at Liquid-Liquid Interfaces

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We investigated the Rayleigh-Plateau (RP) instability at liquid-liquid interfaces by molecular dynamics (MD) simulations. Compared with gas-liquid systems, the present setup avoids evaporation and enables a direct comparison with continuum theory for two fluids with identical viscosities [1]. The system consisted of two immiscible Lennard-Jones liquids with the same physical properties inside and outside a cylindrical interface. We examined cylinders with several initial radii under two conditions: one with an imposed single-mode perturbation and one without any imposed perturbation.

For the perturbed initial condition, the growth rate was evaluated from both the breakup time and the time evolution of the imposed mode amplitude. The dispersion relation estimated from breakup times showed strong finite-size effects, especially for small radii. In contrast, when the growth rate was extracted from the early exponential growth of the imposed mode, the agreement with Stone's linear theory became much better [1]. For the largest radius studied, the simulation reproduced the theoretical dispersion relation well, including negative growth rates in the stable region. This shows that continuum theory can remain valid even for a very small liquid cylinder when thermal fluctuations are effectively suppressed by a controlled perturbation.

For the unperturbed initial condition, we analyzed the breakup dynamics induced by thermal fluctuations. The minimum radius $r_{\min}$ followed the power law $r_{\min} \propto (t_c - t)^\alpha$, where t_c is the breakup time, following the framework commonly used for singular breakup dynamics [2]. The exponent α increased systemati-

cally with the initial cylinder radius, showing that thermal fluctuations become less important as the system size increases. Smaller radii therefore exhibited stronger deviations from macroscopic behavior.

These results show two complementary aspects of microscopic RP instability. With an imposed perturbation, the instability growth follows classical hydrodynamic predictions even for cylinders only several molecular diameters in radius. Without imposed perturbations, the breakup process is strongly affected by thermal fluctuations and finite-size effects. The present study therefore clarifies how continuum-like behavior and fluctuation-dominated dynamics coexist in nanoscale liquid-liquid interfacial instability.

The present liquid-liquid model also provides a useful platform for future studies of microscopic hydrodynamics. Because the physical properties are matched across the interface, deviations from classical theory can be attributed more clearly to thermal fluctuations, finite-size effects, and molecular discreteness. This simplicity should make it possible to quantify the range of validity of continuum descriptions in nanoscale interfacial flows more systematically.

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From Protein Folding Theory to Rational Protein Design

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Many proteins achieve their biological functions only after folding into well-defined three-dimensional conformations. Accordingly, elucidating protein folding mechanisms remains a central challenge in fundamental life science research. In recent years, deep-learning based approaches to protein structure prediction, most notably AlphaFold [1], have been developed, and its development was honored with the 2024 Nobel Prize in Chemistry. However, despite its remarkable success, AlphaFold cannot predict the actual pathways of protein folding.

To address this limitation, we developed a statistical mechanical framework, the WSME-L model, which enables prediction of folding processes for a broad range of proteins [2]. To assess its general applicability, we applied the model to numerous proteins and analyzed their folding pathways. Inter-residue contact energies were estimated using the MM/PBSA module of the AMBER package [3], while free energy landscapes describing protein folding processes were computed using in-house WSME-L

software written in C++ and Python.

Using this approach, we predicted folding pathways for various proteins and validated the results by comparison with experimental data. The WSME-L model successfully distinguished distinct folding behaviors even among structurally similar proteins. We also applied the model to proteins whose folding processes are difficult to investigate experimentally due to highly complex native structures. In particular, we determined the order of structural formation during the folding of laminin and bone morphogenetic protein-2, providing insights relevant to their efficient production for medical applications. Furthermore, we explored extensions of the theory to describe protein-protein interactions, with a particular focus on coupled folding and binding reactions involving intrinsically disordered proteins.

Aldehyde deformylating oxygenase (ADO) synthesizes alkanes equivalent to diesel fuel and is therefore of interest for biofuel production; however, its catalytic activity is very low [5]. We previously showed that ADO

forms a complex with its upstream enzyme, acyl-ACP reductase (AAR), enabling efficient substrate transfer without dissociation [6]. This suggests that strengthening the AAR/ADO interaction could enhance overall alkane production. To test this hypothesis, we rationally designed AAR/ADO mutants with enhanced interactions using the deep learning-based sequence design software ProteinMPNN [7] together with the physics-based protein design platform Rosetta [8]. Experimental validation is currently underway.

Because petroleum-derived products include fuels and plastics, reducing dependence on petroleum requires biological production routes to plastic precursors. Catechol 1,2-dioxygenase (CatA) catalyzes the synthesis of *cis,cis*-muconic acid, a precursor of polyethylene terephthalate. To enhance CatA activity using our original strategy for enzyme activity improvement, we performed molecular dynamics simulations with AMBER [3] and GROMACS [9] to characterize the substrate-bound and product-bound conformations of CatA, and used LigandMPNN [10] to rationally design mutants with improved activity. Several mutants with improved Michaelis constants (K_m) were obtained, and the design of mutants with enhanced turnover numbers is ongoing.

Finally, efficient screening of highly active enzymes in directed evolution experiments requires sensor proteins that emit fluorescence proportional to product concentration. To this

end, we are developing rational design methodologies for fluorescent sensor proteins that specifically recognize product ligands.

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Development of machine-learning force fields to analyze atomic layer processing

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Recently, machine-learning force fields (ML-FFs) have emerged as accurate surrogate models for density functional theory (DFT) calculations, enabling high-fidelity classical molecular dynamics (MD) simulations in materials science. While various ML-FF models successfully simulate thermodynamic equilibrium systems, they often fail in high-energy ion irradiation environments, such as sputtering and etching. In these simulations, high-energy ion impacts force atoms into extreme proximity, causing standard DFT calculations to diverge and rendering the resulting force fields unstable or inaccurate.

To address this limitation, this study couples Ziegler-Biersack-Littmark (ZBL) potential functions to represent short-range repulsive interactions with ML-FFs for longer-range behaviors. The ML-FFs are constructed using Behler-Parrinello Neural Networks (BPNN) and Graph Neural Networks (GNN), optimized via active learning with "query-by-committee" sampling. Specifically, we use the n2p2, Allegro, and SevenNet trained on reference data computed via Quantum ESPRESSO. We apply this framework to Si and SiO₂ systems to

simulate ion beam sputtering and etching. The results demonstrate good agreement with both beam experiments and conventional classical MD simulations. Finally, we also demonstrate the extensibility of this ML-FF framework to chemistry-driven processes, focusing on plasma-enhanced atomic layer etching (ALE) and atomic layer deposition (ALD), including metal oxide and nitride etching using organic precursors,[1] as shown in Fig. 1.

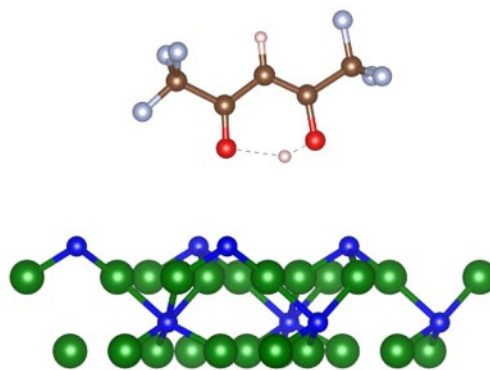


Fig.1 Structure of Hhfac above the Ni₃N surface. (Coloring: dark green – Ni, blue – N, white – F, brown – C, red – O, light pink – H)

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Record-low thermal boundary resistance at bonded GaN/diamond interface by controlling ultrathin heterogeneous amorphous layer

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In semiconductor-on-diamond structures, a non-crystalline buffer layer is required to achieve interfacial bonding due to lattice mismatch, which, however, typically results in high thermal boundary resistance (TBR) and limits device heat dissipation. Interestingly, theoretical studies have suggested that amorphous interfaces can exhibit anomalously low TBR, far below that of their crystalline counterparts. Verifying these predictions and systematically investigating interfacial thermal transport require the fabrication of ultrathin amorphous interfacial layers, yet experimental realization remains highly challenging, thereby limiting related research. Accordingly, this study aims to fabricate ultrathin amorphous interfacial layers and explore their impact on thermal conduction across GaN/diamond interfaces.

We fabricated GaN/diamond samples with varying amorphous interfacial layer thicknesses using a room-temperature bonding method, and measured their TBR via the TDTR technique, as shown in Fig. 1. As the interfacial layer thickness increased from 2.5 nm to 5.3 nm, the TBR rose from 8.3 to 35.0 $\text{m}^2\cdot\text{K}/\text{GW}$. Notably, the TBR of 8.3 $\text{m}^2\cdot\text{K}/\text{GW}$ represents a record

low for directly bonded GaN/diamond interfaces, highlighting its potential significance for efficient thermal management in GaN devices.

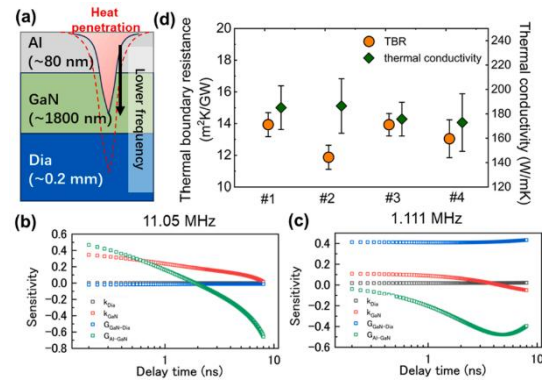


Fig.1 TDTR measurement for GaN-on-diamond system.

(a) Schematic of the modulation frequency-control in tuning the penetration depth of TDTR measurement. Sensitivity calculation results for $G_{\text{Al-GaN}}$, $G_{\text{GaN-Dia}}$, $K_{\text{GaN-Dia}}$ under (b) 11.05 MHz, $G_{\text{GaN-Dia}}=30 \text{ MW}/\text{m}^2\text{K}$; (c) 1.111 MHz, $G_{\text{GaN-Dia}}=30 \text{ MW}/\text{m}^2\text{K}$. (d) Thermal boundary resistance of Al/GaN interface ($R_{\text{Al-GaN}}$) and the thermal conductivity of the GaN layer (K_{GaN}) measured under a modulation frequency of 11.05 MHz.

Furthermore, we investigated the underlying mechanism for the pronounced sensitivity of the TBR to interfacial thickness using molecular dynamics simulations, as shown in Figs. 2 and 3. Theoretical analysis indicates that the diamond/ SiO_x inter-diffusion

layer introduces high-frequency interfacial vibrational modes, whose frequency range extends beyond the primary vibrational spectrum of crystalline diamond, thereby enhancing lattice vibrational mismatch and suppressing phonon transport.

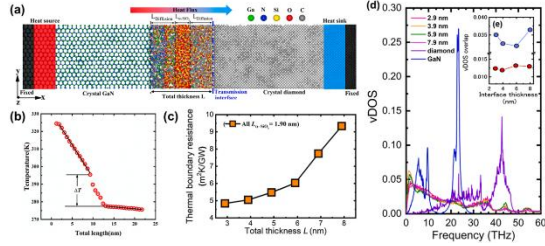


Fig.2 Interfacial heat conduction calculated by MD simulation. (a) Schematic of a typical MD simulations model with a layer-like amorphous interface. (b) Typical temperature profile of the system, where the linear fitting is performed to obtain the difference of temperature at GaN/diamond interface. (c) TBR of GaN/diamond interface with different interfacial thickness; SiO_x layer was fixed to 1.9 nm. (d) vDOS of GaN, diamond, and the entire interfacial layer with a thickness of 2.9, 3.9, 5.9, and 7.9 nm. (e) vDOS overlap between GaN/interfacial layer (blue symbol) and diamond/interfacial layer (red symbol).

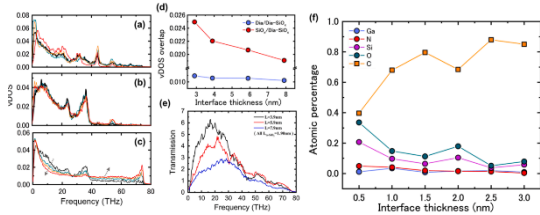


Fig.3 Interfacial vibrational states and heat carrier analysis in MD simulation. vDOS of (a) GaN- SiO_x diffusion region, (b) SiO_x region, and (c) diamond- SiO_x diffusion region; The interfacial layer thicknesses are 2.9 (black), 3.9 (green), 5.9 (orange), and 7.9 nm (red); grey arrow shows the trend in vDOS at individual frequencies

ranges. (d) vDOS overlap between SiO_x /diamond- SiO_x diffusion region and diamond/diamond- SiO_x diffusion region, respectively. (e) Heat carrier transmission at interface near the c-diamond (marked in Fig.2(a)) under different interfacial layer thicknesses. (f) Concentration of individual elements in SiO_x /diamond diffusion layer with different interfacial thickness.

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Numerical Study on the Magnetization Process of the $S=1$ Spin Ladder

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The magnetization plateau has attracted a great deal of interest as a macroscopic quantum phenomenon. Oshikawa et al.[1] derived the rigorous necessary condition for the appearance of the magnetization plateau in the one-dimensional quantum spin systems

$$Q(S - m) = n, \quad (1)$$

where S and m are the total spin and the magnetization per unit cell, respectively, Q is the periodicity of the ground state, and n is a positive integer. The previous magnetization measurement of the organic $S = 1$ spin ladder material[2] 3, 3', 5, 5'-tetrakis(*N*-tert-butylaminoxyl)biphenyl (abbreviated as BIP-TENO), observed a magnetization plateau at 1/4 of the saturation magnetization. According to the rigorous condition Eq.(1), this 1/4 plateau can appear only when the ground state has the two-fold degeneracy due to the spontaneous translational symmetry breakdown. The spin frustration due to the second or third nearest neighbor interaction was proposed[3, 4, 5, 6], but the correct origin of the 1/4 plateau of BIP-TENO has not been clarified[7]. Recently the numerical diagonalization and the density matrix renormalization group analy-

sis indicated the two competing anisotropies can induce the translational symmetry broken magnetization plateau in the $S = 1$ antiferromagnetic chain[8, 9, 10]. Thus it would be interesting to consider the possibility of the translational symmetry broken magnetization plateau based on such competing anisotropies in the $S = 1$ spin ladder system. In the present work we investigated the magnetization process of the $S = 1$ spin ladder with the easy-axis anisotropy at the leg interaction and the easy-plane single-ion one at each site. The numerical diagonalization of finite-size clusters and the level spectroscopy analysis[11, 12, 13, 14, 15] indicated that the translational symmetry broken plateau would appear at 1/4 and 3/4 of the saturation magnetization. In addition the translationally symmetric plateau was revealed to appear at the 1/2 magnetization. The phase diagrams for the two anisotropies at 1/4, 1/2, and 3/4 of the saturation magnetization were obtained[16].

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Magnetization Process of the $S=3/2$ Antiferromagnetic Chain

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The magnetization plateau is one of interesting topics in the field of the condensed matter physics. It was proposed as the Haldane gap which appears in the magnetization process[1]. Based on the Lieb-Schultz-Mattis theorem[2], the rigorous necessary condition for the appearance of the magnetization plateau in the one-dimensional quantum spin systems was derived as the following form[1]

$$Q(S - m) = \text{integer}, \quad (1)$$

where S and m are the total spin and the magnetization per unit cell, respectively, and Q is the periodicity of the ground state. Several magnetization plateaux with $Q = 1$ have been theoretically predicted using some numerical analyses[3, 4, 5, 6, 7, 8], and experimentally observed[9]. The translational symmetry broken magnetization plateaux with $Q = 2$ were also theoretically predicted in several systems[10, 11, 12, 13, 14, 15, 16], based on the mechanism caused by the spin frustration.

The recent work[17] using the numerical diagonalization and the density matrix renormalization group calculation revealed that the $S = 1$ antiferromagnetic chain with the single-ion and coupling anisotropies competing each

other can exhibit the translational symmetry broken magnetization plateau at half the saturation magnetization. Since the double period structure like $|\cdots 101010 \cdots\rangle$ is realized at the plateau, it should be called the Néel plateau. This plateau cannot appear, until $Q = 2$ is realised. On the other hand, the Néel plateau like $|\cdots 202020 \cdots\rangle$ was also theoretically predicted using the numerical diagonalization at half the saturation magnetization of the $S = 2$ antiferromagnetic chain with the same competing anisotropies, although the necessary condition (1) is satisfied even for $Q = 1$ [18]. In the present work, we investigated the $S = 3/2$ antiferromagnetic chain to which the single-ion and coupling anisotropies are introduced in a competing way using the numerical diagonalization of finite-size clusters and the level-spectroscopy analysis. Our purpose is to consider the possibility of the Néel plateau at $1/3$ and $2/3$ of the saturation magnetization. Several $1/3$ plateaux for $Q = 1$ had already been theoretically predicted, while no plateau had been revealed to appear at the $2/3$ magnetization, because $Q = 2$ is necessary. We obtained an extended phase diagram at the $1/3$ magnetization and the initial one at the $2/3$

magnetization[19].

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Critical behavior of measurement induced transition

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Our research over the past year centered on the symmetry classification and spectral statistics of random quantum systems, with a particular emphasis on non-Hermitian Hamiltonians and nonunitary quantum dynamics [1,2]. As a principal achievement in 2025, we studied the entropy dynamics of monitored fermion systems, where continuous quantum measurements are performed on free fermions [3]. This problem is motivated by the recent rapid development of measurement-induced phase transitions, in which unitary time evolution tends to scramble quantum information whereas measurements extract information from the system. The competition between these two processes gives rise to purification dynamics that has no direct counterpart in closed quantum systems. Our purpose was to clarify the universal aspects of this dynamics by focusing on the spectral evolution of Gaussian density matrices.

One of the central results is the derivation of universal Rényi entropy fluctuations in the chaotic regime. These fluctuations are independent of microscopic details of the model and are the nonunitary counterpart of the universal conductance fluctuations known in quantum transport in mesoscopic electronic systems. We also clarified how the fluctuations depend on the fundamental symmetry class of the nonunitary dynamics. The analytical predictions were confirmed by extensive numerical simulations, including dynamics generated by Haar-random unitary matrices and by local Hamiltonians.

The above results provide a useful theoretical basis for further studies of measurement-

induced transitions and for numerical diagnostics based on Lyapunov exponents of quantum trajectories. As ongoing work, we are extending this research in two directions. First, we are applying time-series analysis based on machine-learning techniques, including LSTM and transformer architectures, to entropy dynamics generated by monitored quantum systems. Second, we are investigating the effect of electron-electron interactions on the entropy dynamics using the tensor network technique, with the aim of clarifying which parts of the free-fermion universality survive in genuinely interacting many-body systems.

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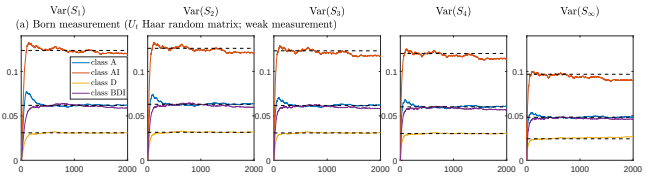


Figure 1: Variance $\text{Var}(S_\alpha)$ of Rényi entropy in the presence of weak measurement with the Haar random unitary dynamics in various symmetry classes. Taken from Ref. [3].

Crystal structure prediction of quaternary oxides based on mathematical crystal chemistry

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Mixed-integer nonlinear programming (MINLP), which has been widely used in process systems engineering, is the optimization problem involving both the continuous and discrete variables. Generalized disjunctive programming (GDP) represented by continuous and Boolean variables is the special case of MINLP, where Boolean variables is just utilized to enforce the constraint on continuous variables. GDP models can be reformulated as MINLP problems using the Big-M or Hull Reformulation [F. Trespalcios *et al.*, *Chemie Ingenieur Technik* **86**, 991 (2014)]. Mathematical crystal chemistry formulates the empirical rules of inorganic structural chemistry as GDP [R. Koshoji, in preparation]. The formalization is based on the concept that crystal structures can be discovered very efficiently if we successfully assume the atomic environment of each atom. The algorithm to solve this problem makes use of two subproblems as done in the Outer-approximation or Generalized Bender Decomposition. For the former subproblem, the Boolean variables are fixed, and accordingly, the continuous optimization problem can be regarded as the dense packing problem of atomic spheres with several radii under the constraints on such as coordination polyhedra and interatomic distances. For the latter subproblem, the continuous variables are fixed, and the Boolean variables are optimized to maximize the number of chemical bonds with satisfying all the constraints on interatomic distances, feasible compositions of coordination polyhedra, and feasible linking of polyhedra.

The algorithm demands tiny data such as atomic

position and Boolean variables designating the type of interatomic-distance constraints, and besides, the algorithm itself is very simple. Therefore, it spends tiny computational time to design crystal structure prototypes. For example, the laptop computer will discover the quaternary oxides of $\text{BaDyFe}_4\text{O}_7$ and VMO_2CsO_8 in one second. The software **MARICI** implementing the algorithm is distributed under the MIT License [3], so you can freely check the computational efficiency on your laptop computer.

The previous studies clarifies that at least most of oxides registered in database can be regarded as optimal solution of GDP, and besides, the algorithm can discover a wide variety of ionic crystal structures such as spinel, pyrochlore (α and β), pyroxene, quadruple perovskite, $\text{YBa}_2\text{Cu}_3\text{O}_7$, and LaFeAsO [1-2]. Note that some of them can be designed as unique optimal solution.

An exhaustive search for crystal structures of quaternary oxides $\text{A}_k\text{B}_l\text{C}_m\text{O}_n$ and $\text{A}_k\text{B}_l\text{D}_m\text{O}_n$ discovers a wide variety of structural prototypes. The constraints for each cation is listed below.

- Cation A: $r^{(I)} = 0.32$, $R^{(I)} = 0.32$, $R^{(R_I)} = 1.4$, $c_i^{(I,O)} = 4$, $C_i^{(I,O)} = 4$
- Cation B: $r^{(I)} = 0.60$, $R^{(I)} = 0.60$, $R^{(R_I)} = 1.4$, $c_i^{(I,O)} = 6$, $C_i^{(I,O)} = 6$
- Cation C: $r^{(I)} = 1.40$, $R^{(I)} = 1.40$, $R^{(R_I)} = 1.8$, $c_i^{(I,O)} = 9$, $C_i^{(I,O)} = 12$
- Cation D: $r^{(I)} = 0.80$, $R^{(I)} = 1.30$, $R^{(R_I)} = 1.8$, $c_i^{(I,O)} = 8$, $C_i^{(I,O)} = 8$

The number of chemical composition is 3055 if k, l, m, n are constrained as

$$1 \leq k + l + m + n \leq 25$$

$$\frac{1}{7} \leq \frac{l}{k}, \frac{k}{l}, \frac{m}{k}, \frac{k}{m}, \frac{l}{m}, \frac{m}{l} \leq 7.$$

Among them, the optimal solutions are discovered in about 350 kinds of chemical composition. Although the number of optimal solutions for each chemical composition obtained by mathematical crystal chemistry tends to be very small, it is difficult to execute *ab-initio* simulation for all the optimal structures for evaluating structural stability due to too many chemical compositions. Therefore, I must pick up promising crystal structures from them to predict synthesizable materials. At first, I select crystal structures consisting of the smaller number of wyckoff positions, and I evaluated the formation enthalpies of them. Accordingly, I found several materials whose formation enthalpies per atom are less than 0.1 eV/atom compared to the several experimentally known decomposition mixtures.

I should note that the software **MARICI** also implements the algorithm to create chemical bonds based on Voronoi polyhedra, which is also formulated by GDP. Accordingly, I confirmed that only one type of crystal structure (e.g. $\text{CeP}_2\text{Al}_3\text{O}_{14}$) makes the kagome lattice of octahedra via edge or face sharings among the $A_kB_lC_mO_n$ and $A_kB_lD_mO_n$ crystal structures. Since I successfully discovered new crystal prototypes with kagome lattice, we can expect that mathematical crystal chemistry will find many unknown crystal structures with exotic quantum phenomena.

Furthermore, the algorithm to calculate Eward Sum is also implemented in the software **MARICI**. To remove most of unpromising crystal structures from all the optimal solutions, at first I calculate the Löwdin charge of each cation in the simple binary compounds by the software **LOBSTER** [Peter C. Müller *et al.*, J. Phys. Chem. C **125**, 7959 (2021)]. Next, the atomic charges are assigned to all the cations to calculate Madelung energies to estimate the structural stability. Accordingly, I found that some of the crystal structures have negative Madelung energy compared to the convex hull

consisting of the Madelung energies of experimentally known materials. The “promising” structures do not necessarily have high symmetry or consist of small number of wyckoff positions. The result shows that the estimation of structural stability by the classical model is effective. The AI techniques are considered to be more robust and effective to select promising structures, but I plan to make finishing mathematical crystal chemistry as the extension of inorganic structural chemistry without AI techniques.

Finally, we can suggest the new computational scheme to predict unknown materials. First, the feasible atomic environments of each atom is assumed. Second, crystal structure prototypes are dicovered by solving GDP. Third, atomic charges of atoms are evaluated to calculate Madelung energy. Fourth, we remove most of unstable structures with respect to Madelung energy. Fifth, we execute *ab-initio* simulation to confirm the structural stability. We will show that this scheme is very effective by succeeding in synthesizing new oxides with experimentalists based on mathematical crystal chemistry.

Now I collect many data of crystal structure prototypes. I will continue to use the supercomputer of ISSP, and I plan to write a few papers in the academic year of 2026.

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Study on structure-properties relationship in uniform/dynamic polymer networks via precise graph structure analysis.

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Introduction

Polymer gels and cross-linked rubbers are widely used materials that exhibit both flexibility and toughness. However, their network structures are heterogeneous, making it difficult to quantitatively describe their mechanical properties based on structure. In particular, the quantitative impact of cross-links and structural defects on elasticity remain poorly understood. Recent approaches to improving mechanical performance include the homogenization of strand lengths and the introduction of dynamic cross-links. Nevertheless, clear molecular design principles have not yet been established.

In our previous work, we developed a graph-based structural analysis algorithm for tetra-/tri-PEG like networks (SPNs) enabling the extraction of elastically effective cross-links and strands and the quantitative prediction of elastic modulus [1]. However, the general applicability of this method to other networks remains unclear.

In this study, we apply coarse-grained molecular dynamics simulations and graph-based structural analysis to TPNs (Fig. 1.) to elucidate the effective network for elasticity.

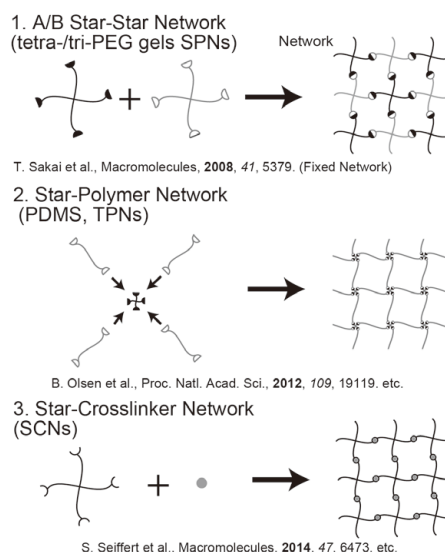


Fig.1. Schematics of TPNs, SPNs, SCNs

Computational Methods

Uniformly cross-linked PDMS-like networks (Telechelic Polymer Networks, TPNs) with tri- and tetra-functional junctions were constructed, and their mechanical properties were systematically evaluated. The developed graph-based analysis method was applied to extract effective network structures.

For comparison, tetra-PEG/tri-PEG networks (Star Polymer Networks, SPNs) and networks formed via star-shaped macromers and crosslinker molecule (Star Crosslinker Networks, SCNs) were also constructed.

Each system consisted of approximately

100,000 particles. After sufficient equilibration and cross-linking reactions, uniaxial stretching simulations were performed along three directions at a constant strain rate ($10^{-6} \tau^{-1}$), and stress-strain curves were obtained. Excluded-volume interactions were introduced in all simulations.

Results and Discussions

(1) Comparison between SPNs and TPNs

The elastic modulus calculated from the density of effective strands and junctions using the phantom network model was compared with simulation results. Both SPNs and TPNs exhibited a scaling relationship with a slope of approximately 2 [3].

TPNs showed lower modulus values than SPNs. This difference originates from the formation of primary loop structures, which remain as elastically inactive defects in TPNs, whereas in SPNs such structures can be transformed into effective strands during network formation [3].

Consistently, simulations of dynamic cross-linked elastomers revealed that the elastic modulus initially increases and subsequently decreases over time, accompanied by a conversion of intermolecular cross-links into intramolecular ones [4]. This transition leads to an increase in loop-like, elastically inactive structures, supporting the interpretation that loop formation governs the reduction in elasticity.

However, TPNs showed lower modulus values than SPNs. This difference originates from the formation of primary loop structures, which remain as elastically inactive defects in TPNs, whereas in SPNs such structures can be transformed into effective strands during network formation [3].

(2) Comparison between TPNs and SCNs

Stress-strain curves were compared by varying strand length, functionality, and cross-linking density. For identical strand length and functionality, TPNs and SCNs exhibited nearly identical mechanical responses. (Fig. 2. as an example) This suggests that when network strand length is equivalent, effective network structure does not depend on relative size of multifunctional/bifunctional precursors.

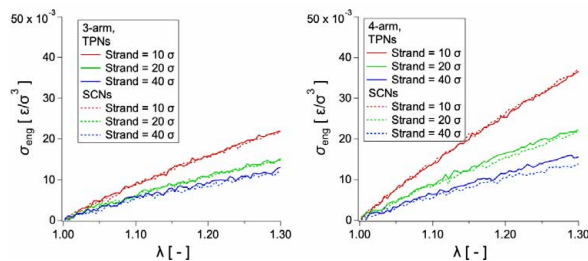


Fig. 2. Stress-elongation curves of TPNs and SCNs with conversion = 0.96 at various network strand lengths and number of branches.

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MD Simulations on Single-Molecule Reactors based on Bottlebrush Polymers

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Introduction

Bottlebrush polymer reactors (BBPRs), recently developed by Nakagawa et al., are nanoscale reactors for polymerization constructed by grafting substrate monomers and long side chains onto a polymer backbone[1]. Owing to the excluded-volume effect of the side chains, intermolecular polymerization is suppressed, while catalyst molecules can freely penetrate the brush region and react with substrate monomers. As a result, substrates are locally concentrated within the brush, enabling precise intramolecular polymerization within a single molecule [1]. However, the molecular mechanism underlying this process remains unclear, so computational investigation is required.

In this study, we constructed a coarse-grained model of BBPRs, then analyzed static property and reaction kinetics using coarse-grained molecular dynamics simulations using various brush and main chain lengths. The resulting structures and reaction efficiencies were systematically evaluated.

Calculation Methods

Polymer backbones and grafted chains

were modeled using the Kremer–Grest bead–spring model, where approximately five to six carbon atoms were coarse-grained into a single bead. Nine systems were prepared with backbone lengths of 50, 100, and 200 beads and side-chain lengths of 10, 20, and 40 beads. The ratio of monomer to brush segments in the side chains was set to approximately 1:1. The number of initiator beads are set as 1/5 of monomer beads.

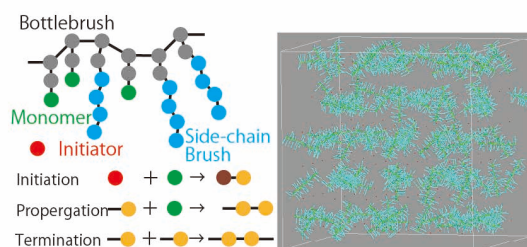


Fig.1. Reaction protocols of BBPRs and snapshot of a system.

First, equilibrium simulations were conducted in the dilute regime to evaluate the radius of gyration R_g , from which the overlap concentration ϕ^* was estimated. Subsequently, 23–266 molecules were introduced into the simulation box to maintain a total particle number of approximately 100,000. Reaction conditions were implemented via kinetic Monte

Carlo simulations (Fig.1.). The molecular weight distributions after reaction were analyzed to elucidate the shielding effect of the brush architecture.

Results and Discussion

After sufficient equilibration in the dilute regime ($\phi=0.0085\sigma^{-3}$) the mean-square radius of gyration $\langle R_g^2 \rangle$ was evaluated, and the overlap concentration was defined as:

$$\phi^* = \frac{3N_{br}}{4\pi \langle R_g^2 \rangle^{\frac{3}{2}}}$$

Where N_{br} is the total number of beads per bottlebrush molecule. The resulting ϕ^* values ranged from 0.04 to 0.15 across all systems. Based on this, reaction simulations were performed in the semidilute ($\phi=0.085\sigma^{-3}$) and melt ($\phi=0.85\sigma^{-3}$) regimes, and reaction kinetics were analyzed over $10^4\tau$

In the concentrated regime, intermolecular polymerization dominated, leading to gelation of the entire system into a single macromolecule. In contrast, in the semidilute regime, polymerization behavior depended strongly on the side-chain length.

The average degree of polymerization of brushes was defined as N_w/N_{br} , where N_w is the weight-average molecular weight. As shown in Figure 2, the average degree of polymerization decreased with increasing side-chain length, while it was less sensitive to backbone length. This indicates that longer side chains effectively shield intermolecular reactions and promote

intramolecular polymerization, consistent with experimental observations.

Conclusion

In this study, bottlebrush polymer reactors (BBPRs) were investigated using coarse-grained molecular dynamics simulations. By systematically varying brush length and concentration, we demonstrated that the excluded-volume effect of the brush suppresses intermolecular reactions and promotes intramolecular polymerization, resulting in narrower molecular weight distributions.

Although free-radical polymerization was considered in this work, extending the analysis to living radical and condensation polymerizations is expected to further establish the general applicability of this reactor concept.

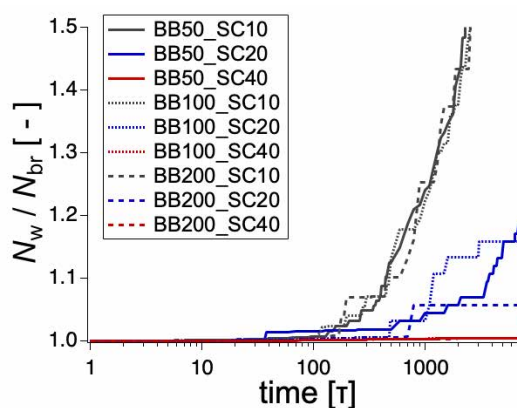


Fig. 2., Reaction time dependence of the average degree of polymerization, bottlebrushes with main chain length = x, side-chain length = y is labeled as BBx_SCy

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Molecular dynamics simulation of disease-causing protein aggregates

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Protein aggregates such as oligomers and amyloid fibrils cause more than 40 diseases. For example, Alzheimer's disease is caused by aggregated amyloid- β (A β) peptides. We have performed molecular dynamics (MD) simulations to understand the aggregation and disaggregation mechanisms of A β peptides.

Recent studies have revealed that the aggregation propensity of A β peptides depends on the curvature of the cell surface. Specifically, A β peptides tend to aggregate more readily as the radius of curvature decreases. However, the underlying mechanism remains unclear. Since Prof. Noguchi at ISSP is an expert in membrane simulations, we initiated a collaborative study with him to elucidate how membrane curvature influences A β peptide aggregation.

First, a lipid bilayer and an aqueous NaCl solution were placed in a simulation box, and molecular dynamics simulations were performed. During the simulation, when the system was gradually compressed laterally while maintaining a constant volume, the membrane suddenly bent at a certain point, and buckling behavior was observed. We generated

highly curved membranes in this way. We then placed A β peptides on them, and are currently continuing molecular dynamics simulations (Figure 1). In parallel, we are also performing simulations of A β peptides on flat lipid bilayers without buckling.

We plan to analyze structural changes in A β peptides induced by membrane interactions and to elucidate the mechanism by which membrane curvature affects the aggregation propensity of A β peptides.

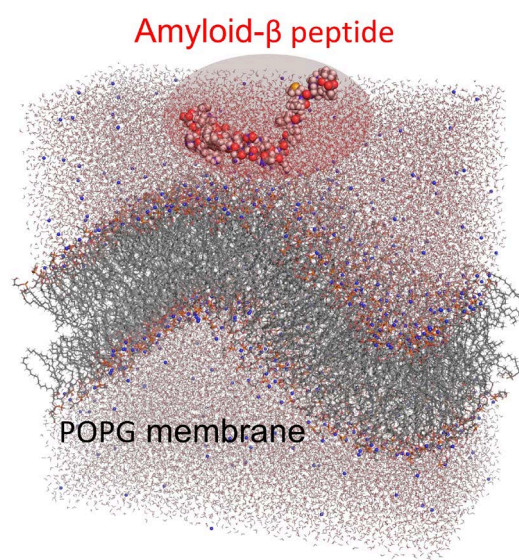


Fig. 1: Molecular dynamics simulation of amyloid- β on POPG membrane.

Dynamics of active Potts models with factorizable numbers of states

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We simulated the nonequilibrium dynamics of q -state active Potts models in square and hexagonal lattices [1–4]. A cyclic flip consumes energy (state $s = 0 \rightarrow 1 \rightarrow 2 \rightarrow 0$ in the three-state Potts model). At low and high flipping energy, the homogeneous cycling and wave modes occur, respectively, for $q \in \{3, 8\}$ at cyclically symmetric conditions. We found that several modes with factorized symmetry additionally emerge when q is factorizable [1]. For example, the modes shown in Fig. 1 are obtained at $q = 6$. In particular, three even- or odd-numbered states ($s = 0, 2, 4$ or $s = 1, 3, 5$) can form domains of spiral waves with two different parameter regions [Fig. 1(c) and (d)]. They rotate forward ($s = 1 \rightarrow 3 \rightarrow 5 \rightarrow 1$) and backward ($s = 1 \rightarrow 5 \rightarrow 3 \rightarrow 1$) directions owing to the stability of the minor three states at the domain boundaries (green domains are inside of red domains in Fig. 1(c) but outside in Fig. 1(d)) [4]. Nucleation and growth at the domain boundary play an essential role in these three-state spiral waves.

When the diagonal states (e.g., $s = 0$ and 3) have attractions, the diagonal states are mixed. The three mixed domains can form spiral waves as shown in Fig. 1(e). When mixed states cover the entire lattices, the dominant two states cyclically change [Fig. 1(f)].

We revealed that the transition between three-state wave and six-state mixing modes is second-order, and its scaling exponents are modified from the equilibrium values [1]. In contrast, the transition between the homogeneous cycling and mixing modes of three states is also second-order, but no change is detected in the exponents. Moreover, a first-order transition is obtained between the waves of three even- or odd-numbered states under asymmet-

ric contact energies, as in the Ising model under a magnetic field [4].

During coarsening from a random mixture to a uniform equilibrium phase in Potts models, the domain length grows proportionally to $t^{1/2}$, following the Lifshitz–Allen–Cahn law. We found that the growth exponent transiently increases slightly before the saturation to spiral waves in the active Potts models [3]. The transient increase is greater at higher q . The coarsening to the three-state waves at $q = 6$ exhibits similar domain growth to that in the three-state active Potts model. We also confirmed that the choice of lattice type (square or hexagonal) and update scheme (Metropolis or Glauber) does not alter the dynamic behavior.

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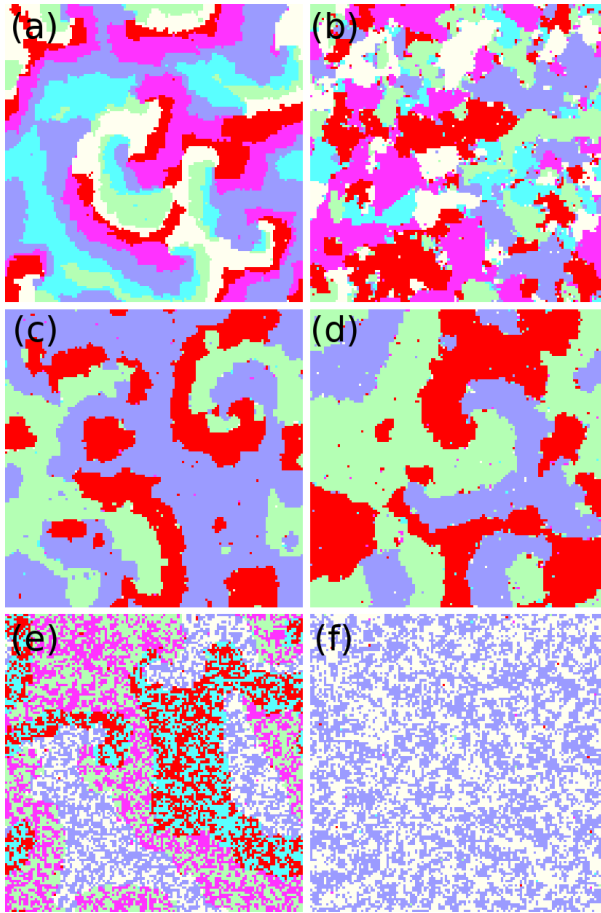


Figure 1: Snapshots of the active six-state Potts model [1]. (a) Spiral waves. (b) Disordered waves. (c) Forward waves of three states. (d) Backward waves of three states. (e) Waves of three domains comprising two diagonal states. (f) Homogeneous cycling of mixed diagonal states. The light yellow, light green, cyan, blue, magenta, and red sites (light to dark in grayscale) represent $s = 0, 1, 2, 3, 4$, and 5 , respectively.

Efficient sampling simulation of the soft modes significantly that contributes to protein properties

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Lysine acetylation is a critical, reversible post-translational modification that modulates protein functions by altering local charge and conformation. Among the enzymes regulating this process are sirtuins, such as the NAD⁺-dependent deacetylase Sir2, which play essential roles in stress resistance, energy metabolism, and aging. A major target for Sir2 is the tumor suppressor protein p53, particularly its C-terminal domain where acetylation at residue K382 regulates transcriptional activity and stability. Although the binding of p53 to Sir2 has been structurally characterized, the precise regulatory role of the conserved cofactor-binding loop in facilitating NAD⁺ entry remained poorly understood.

To investigate the loop dynamics, we employed a combination of conventional molecular dynamics and parallel cascade selection molecular dynamics simulations [1] to capture rare conformational transitions. These advanced techniques allowed for the characterization of the conformational space occupied by apo Sir2 as well as complexes bound to either acetylated or nonacetylated p53

[2]. By defining specific surface areas at the entrance of the NAD⁺-binding pocket as shown in Fig. 1, the study was able to quantitatively distinguish between various open and closed states of the enzyme. The simulations revealed that the cofactor-binding loop acts as a flexible ceiling for the binding pocket, directly influencing the accessibility of NAD⁺.

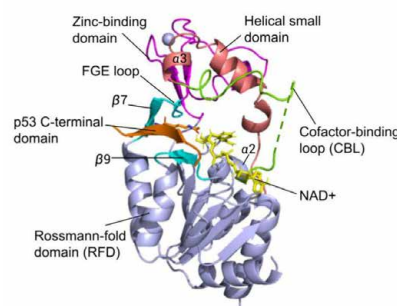


Fig. 1: The structure of the Sir2-Af2 complex with acetylated p53.

The findings suggest that the acetylation status of p53 exerts a profound allosteric influence on the structural state of Sir2. Specifically, the binding of acetylated p53 was found to drive the cofactor-binding loop into an open conformation, which significantly expands the entrance to the NAD⁺-binding

pocket and facilitates the deacetylation reaction. Conversely, when Sir2 is bound to nonacetylated p53 or exists in its apo form, it predominantly adopts closed conformations that naturally impede the entry of NAD⁺. This indicates that the presence of the acetyl group on the substrate is the key signal that triggers the enzyme's transition into a catalytically receptive state.

This sequential regulation is characterized as a tandem allosteric effect, where both the reactant and the product contribute to the efficiency of the catalytic cycle. Initially, the forward allosteric effect of the reactant promotes cofactor binding by opening the pocket to allow NAD⁺ entry. Following the deacetylation of p53, the resulting product exerts a reverse allosteric effect that drives the pocket toward a closed state. This closure likely prevents the rebinding of inhibitors like nicotinamide and facilitates the release of reaction products, thereby preventing the reverse reaction and accelerating the overall cycle.

Analysis of entropy transfer pathways identified how the allosteric signal from residue K382 of p53 travels through the Sir2 structure to reach the distant cofactor-binding loop as shown in Fig 2. The communication involves multiple interconnected routes passing through the Rossmann-fold domain, the helical small domain, and the zinc-binding domain. Many of the residues involved in these signaling

pathways, as well as those stabilizing the open and closed states, are highly conserved across species ranging from archaea to humans. This conservation suggests that the tandem allosteric mechanism is a universal feature of the Sir2 family, providing a fundamental framework for their biological functions.

These insights into the molecular mechanisms of Sir2 opening and closure have significant implications for drug discovery and disease intervention. Understanding how to specifically target the closure mechanisms of the NAD⁺-binding pocket could lead to new classes of inhibitors that obstruct NAD⁺ binding, offering alternatives to traditional pocket-occupying drugs.

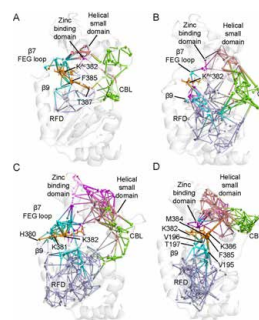


Fig. 2: Allosteric communication pathways from K^{Ac}382/K382 to the CBL during the opening and closure processes of the NAD⁺-binding pocket. (A) S1 opening. (B) S2 opening for Sir2/K^{Ac}382-p53. (C) S1 closure. (D) S2 closure for Sir2/p53.

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Nonlinear particle-continuum switching in multiscale Smoothed-Particle Hydrodynamics (SPH) method

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There are two regions in a complex polymeric flow around an obstacle, i.e. the bulk flow region and the boundary layer region near the obstacle surface. We have been developing an “embedding-type multiscale simulation” where the macroscopic flow is simulated using smoothed particle hydrodynamics (SPH) simulation where the local constitutive relation is determined by microscopic simulator (MicS) embedded in each of the SPH particles. For an accurate evaluation of the local stress field, we usually embed a molecular dynamics (MD) simulator as MicS. As the use of such molecular dynamics simulators requires a large amount of computational resources, it is desired to accelerate the simulation by switching the MD simulator with a much faster simulator such as an analytic constitutive model when the local stress is less than a threshold value. In Ref.[1], we applied such a switching technique between MD simulator and a linear viscoelastic constitutive model in the boundary layer near the obstacle.

In highly nonlinear and non-Markovian complex viscoelastic and elastoplastic flows, however, the use of the linear constitutive model is not enough to realize a high efficiency of the switching technique. Therefore, we

developed a switching technique using nonlinear constitutive model and applied it to a MicS composed of nonlinear dumbbell molecules bonded with an FENE (finite extensible nonlinear elastic) spring [2]. Figure 1 shows a comparison between a switching technique using linear constitutive model (Fig.1(a)) and that using nonlinear constitutive model (Fig.1(b)). Shown are the time evolution of the local normal stress of a system under an external oscillatory elongation and compression deformation, where the red data were calculated with constitutive model and the green data with MD simulations. While linear constitutive model shows discontinuity at the switching time, the nonlinear constitutive model can be smoothly connected to the MD simulation. It is also confirmed that the linear

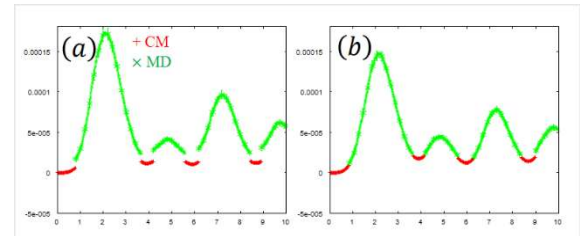


Figure 1: Time evolution of the normal stress under a periodic elongation and compression deformation simulated with a switching technique using (a) linear constitutive model and (b) nonlinear constitutive model, respectively.

constitutive model overestimates stress while the nonlinear one does not.

Figure 2 shows a snapshot of a flow near a surface of a cylindrical obstacle (bottom right) simulated with the nonlinear switching technique, where the parameters of the nonlinear dumbbell molecules in the MD simulation are chosen so that the dumbbell corresponds to a DNA. In this figure, white SPH particles are those with nonlinear constitutive model and non-white SPH particles are those with embedded MD simulators. The color legend shows the trace of the deviation of the bond orientation tensor from its equilibrium value, i.e. unit tensor. This figure shows that the nonlinear switching can successfully

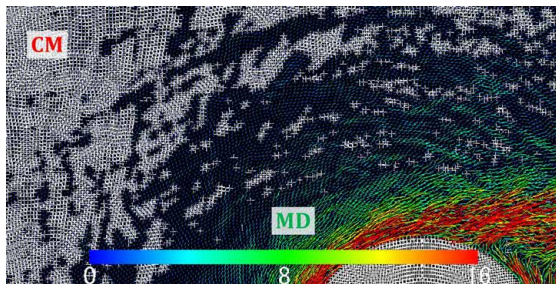


Figure 2: A snapshot of a flow near a cylindrical obstacle.

simulate the polymeric flow near the obstacle.

Acknowledgement

The computation in this work has been done using the facilities of the Supercomputer Center, the Institute for Solid State Physics, the University of Tokyo.

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Molecular dynamics simulation studies of soft matters

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We systematically investigated the nonlinear rheology of equi-weight blends of ring and linear polymers under uniaxial elongational flow by coarse-grained molecular dynamics simulations, and identified for the first time the threshold chain length for the emergence of stress overshoot [1]. Using flexible Kremer-Grest chains ($N_e \approx 80$, $N_{tot} \approx 600,000$), we varied the number of entanglements $Z = N/N_e = 1, 2$, and 4 . The shorter chains ($Z \leq 2$) exhibited only monotonic stress growth, whereas a clear stress overshoot emerged at $Z \approx 4$. Stress decomposition, a topological analysis based on the Gauss linking number, and a conformational analysis revealed that at the threshold chain length each ring is penetrated on average by three to four linear chains, and that this “multiple threading” state excessively stretches the rings, giving rise to the stress peak via subsequent unthreading. Previously, stress overshoots in ring-linear blends had been reported only for highly entangled systems ($Z \approx 14$), which are difficult to synthesize and purify. Our finding that the phenomenon already appears at $Z \approx 4$ lowers the experimental hurdle substantially, since moderately entangled rings are much more accessible via liquid

chromatography at the critical condition (LCCC). We also predicted two-dimensional SANS patterns as a direct structural signature of the thread-to-unthread transition, providing a concrete route for experimental validation. These results were available on arXiv [1].

In NEMD simulations of elongational flow, the simulation box deforms with the flow and the minimum image distance eventually vanishes. For planar elongation, the Kraynik-Reinelt (KR) boundary conditions [3] give a time-periodic lattice, but no such time-periodic lattice exists for uniaxial or biaxial elongation with real-eigenvalue automorphisms [3]. Dobson [4] proposed the generalized KR (g-KR) boundary conditions using two commuting automorphisms to keep the lattice deformation bounded; our existing code UEFEX [2] is based on this framework. More recently, Dobson and Geraldo [5] proposed the Rotating KR (R-KR) boundary conditions, which use a single automorphism with complex conjugate eigenvalues, are time-periodic up to a rotation for uniaxial and biaxial flows, and analytically give a larger minimum image distance than g-KR. However, Ref. [5] presented only the concept and algorithm; no actual MD

implementation had been reported. In this work, as the first implementation of the R-KR method in an MD code, we developed a new LAMMPS plugin that supports R-KR for uniaxial/biaxial elongation and KR for planar elongation (Figs. 1 and 2).

To validate the implementation, we compared the LAMMPS + KR/R-KR results with those of UEFEX [2] for Kremer-Grest polymer melts under identical conditions. As shown in Fig. 3, the stress-strain curves from the two codes agree within statistical error for uniaxial, biaxial, and planar elongations, providing the first numerical demonstration that R-KR works correctly in actual NEMD simulations. Combined with the extensive potentials and parallelization of LAMMPS, the plugin now enables large-scale NEMD simulations of all three elongational flow geometries. The larger minimum image distance of R-KR is especially beneficial for ring-linear blends with extended rings, which we plan to exploit for higher-Z systems and various mixing ratios beyond Ref. [1]. The packages (KR and R-KR) will be released on GitHub [6].

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Hencky strain = 5.00

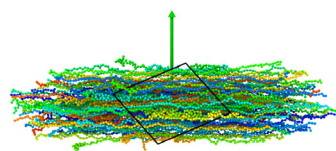
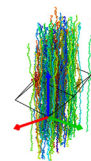


Fig. 1: KR boundary condition for planar elongation

Hencky strain = 5.00



Hencky strain = 5.00

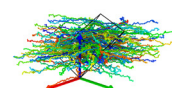


Fig. 2: R-KR boundary condition for uniaxial elongation (left) and biaxial elongation (right).

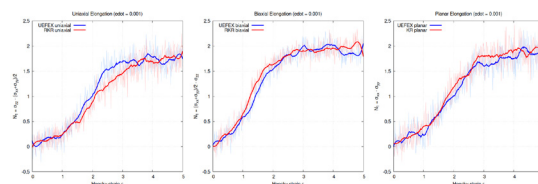


Fig. 3: Comparison of stress-strain curves between UEFEX and R-KR for uniaxial (left) and biaxial (center) elongations and between UEFEX and KR for planar (right) elongation.

Creating a quantum computing database for sensor materials

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Over the past decade, quantum-computing hardware has advanced substantially. Although noise remains a major challenge, the field is entering a regime in which classical emulation is becoming increasingly difficult. There is also growing interest in tackling difficult real-world problems through hybrid quantum-classical approaches that combine quantum computers with high-performance computing (HPC). In such a context, our research focuses on developing hybrid quantum-classical methods for materials simulation, particularly for sensor materials. This includes machine-learning approaches that use results from quantum computers, as well as the development of sampling-based algorithms.

In the past year, we applied the framework of Sakka et al. [arXiv:2504.07396], which uses large language models to automatically generate, evaluate, and refine quantum feature maps for quantum machine learning, to materials systems. Using a quantum kernel method, we designed quantum feature maps that enable efficient and accurate modeling of real-world chemical data, such as NMR chemical shifts.

Another line of our work concerns QSCI (Quantum-Selected Configuration Interaction), a representative sampling-based algorithm that we previously developed. QSCI

uses samples obtained from a quantum computer to identify important electron configurations and then diagonalizes the electronic-structure Hamiltonian in the resulting subspace on classical computers. The method is well suited to quantum-HPC workflows, and its applications have been expanding both in Japan and internationally. For example, IBM provides the QSCI functionality through its Qiskit addon as the sample-based quantum diagonalization (SQD) package. We have recently developed a method that effectively doubles the number of spatial orbitals accessible to QSCI by restricting the space sampled on the quantum computer to the seniority-zero space, in which spatial orbitals are either doubly occupied or empty [arXiv:2602.07912]. This approach was then combined with the QSCI-AFQMC method that we reported last year, yielding a DOCI-QSCI-AFQMC workflow. The resulting workflow was evaluated on the H_6 chain, N_2 dissociation, and the addition of singlet oxygen to a BODIPY dye. Calculations were also carried out on actual quantum hardware, yielding quantitatively meaningful results. Together, these developments provide methodological foundations for building a quantum-computing database for sensor-materials research.

Investigation of Unknown Ice Phases Using Large-Scale Metadynamics Simulations with Unsupervised Machine Learning

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Ice polymorphism is an important research subject, because it plays important roles in the Earth's environment, our daily life, and industry. Recently, a new amorphous ice phase, which has an intermediate density between high- and low-density amorphous ice phases, was discovered experimentally [1], implying the existence of many other unknown ice phases.

In this project, a molecular dynamics (MD) simulation was conducted to search for unknown ice phases. To determine whether amorphous ice phases, which are detected with the MD simulation, correspond to unknown ones, the structure of those phases were analyzed with a method of unsupervised machine learning [2]. To check whether those phases correspond to local minimum ones, an MD simulation combined with the metadynamics (MTD) method (MTD simulation) [3] was also carried out.

The MD simulation was performed for an amorphous ice phase, which was created by quenching a liquid water phase at 1 atm and every 100 atm in the pressure range of 0–3000 atm. The interaction between pairs of water molecules was calculated using the TIP4P/Ice

model. The simulation was carried out with DL_POLY 2.20 [4], in which PLUMED 1.3 [5] was implemented, using System C of ISSP Supercomputer Center.

Results of the analysis with the unsupervised machine learning method indicated that the structure of amorphous ice phase changed around 1500 atm. The density of amorphous ice as a function of pressure also showed a discontinuous change around 1500 atm. A free energy surface obtained with the MTD simulation showed a few shallow minima, implying the existence of a few different amorphous ice phases.

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A Metadynamics Simulation Study on the Mechanism of Ice VI Formation

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According to a phase diagram of water, ice VI is stable at pressures higher than 0.96 GPa at 298 K. However, Lee et al. observed the formation of ice VII in the stability region of ice VI [1]. The reason for it remains elusive. Therefore, in this project, a molecular dynamics (MD) simulation based on the metadynamics (MTD) method (hereafter, MTD simulation [2]) was conducted to resolve this reason.

The MTD simulation was performed for a rectangular-parallelepiped system consisting of 2880 water molecules. The interaction between pairs of water molecules was calculated using the TIP4P/Ice model. The volume of the system was maintained to reproduce the equilibrium density of liquid water at 298 K and 2.12 GPa in the TIP4P/Ice model. Following a previous study [3], two discrete oxygen-oxygen radial distribution functions represented by Gaussian window functions were used as collective variables. The MTD simulation was carried out with DL_POLY 2.20 [4], in which PLUMED 1.3 [5] was implemented to permit combination with the MTD method, using System C of ISSP Supercomputer Center.

Simulation results indicated the formation of a liquid water phase that had a different

structure from that of the equilibrium liquid water at 298 K. A free energy surface obtained with the MTD simulation indicated a shallow local minimum at the position of this phase, suggesting the detected phase was a metastable one. Pair-distribution functions and angular distribution functions were analyzed for this detected phase. Results of the analysis indicated that the arrangement of water molecular oxygen atoms was in a highly ordered state like ice VII. We speculate that this detected phase is related to the formation of ice VII in the stability region of ice VI.

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Machine Learning and Molecular Dynamics Simulation-Assisted Structural Optimization of Carbon Nanotube Yarns

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In this study, molecular dynamics (MD) simulations were used to model carbon nanotube yarns (CNTYs) under tensile loading. The nominal strength — defined as the strength of a CNTY accounting for its hollow core — was used as the optimization objective. Approximately 100 models with varying structural parameters were simulated across multiple supercomputers, including ISSP at the University of Tokyo. Each model was simulated three times, yielding around 300 data points comprising structural parameters and nominal tensile strength values. Based on these results, machine learning optimizations were conducted to identify the combination of structural parameters that yields the highest nominal tensile strength. A parametric study was also carried out to understand the relationships between various parameters and their impact on CNTY strength.

The MD simulations were conducted primarily using Python-based input scripts[1] and run on Supercomputer System B (Ohtaka) at ISSP. For each model, the base files were first prepared on a local computer. Once the model build was complete, the base files were uploaded to ISSP, where LAMMPS was executed using those files as input. Each model typically

required 512 nodes with a 100-hour wall time, using the L4cpu partition. Upon completion of the MD simulations, post-processing was performed on a local computer to conserve the computational quota at ISSP. The post-processing stage extracted the relevant data from each simulated model, including the nominal tensile strength and the simulated twist angle. The simulations yielded nominal tensile strength data for CNTYs with different structural parameters, which served as the training dataset for subsequent machine learning-based structural optimization.

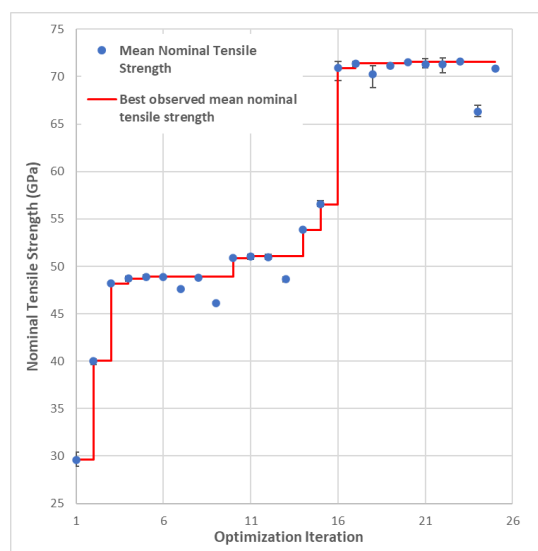


Figure 1. Plot of the main optimization generation vs the nominal strength of CNTY

The main optimization revealed that the optimal CNTY structure is characterized by an

armchair configuration, a small inner tube diameter, a low wall count, near-zero crosslink density between walls, and a low twist angle. Compared to our previous parametric study[1], the optimization favored a wall count of 2 with no interwall crosslinks. This is attributed to the fact that crosslinks introduce defects in the CNTY wall, thereby reducing nominal tensile strength. The progression of nominal tensile strength across the main optimization generations is shown in Figure 1.

To further investigate the relationship between crosslink density and nominal tensile strength, a separate machine learning optimization was conducted on a 5-wall CNTY group, following the same procedure but with the wall count fixed at 5. The crosslink densities between walls were varied from 0.00% to 1.90%. This optimization retained the preference for a small inner wall diameter and a low twist angle. However, in the 5-wall case, models with interwall crosslink densities above 1.00% tended to yield higher tensile strength. From these findings, it was concluded that in multi-wall CNTYs with a high wall count and large inner wall diameter, a high crosslink density is preferable to facilitate interwall load transfer. When the outer wall fails, the load is transferred to the next inner wall via crosslinks acting as anchors. Figure 2 shows the trade-off between outer wall diameter (determined by inner wall diameter) and the presence of crosslinks. At low

outer wall diameters, the no-crosslink scenario is preferable for achieving high tensile strength. However, beyond a certain outer wall diameter, the presence of crosslinks becomes increasingly beneficial for load transfer, ultimately yielding higher nominal tensile strength than the no-crosslink case.

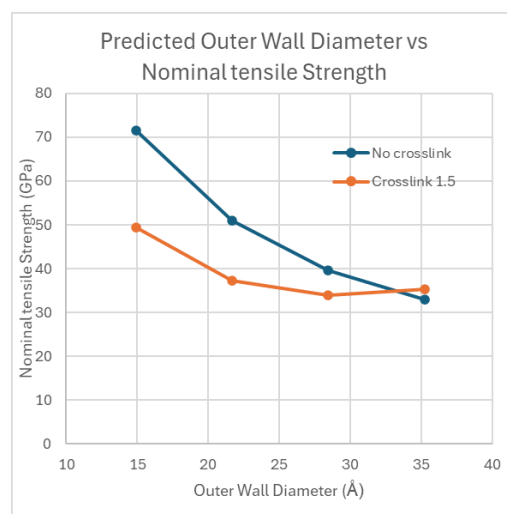


Figure 2. Trade-off graph between the no-crosslink CNTY and CNTY with 1.50% crosslink density, considering the outer wall diameter.

The results of this study will be reported in a manuscript following the completion of the next optimization for 10-degree twist angle CNTYs. The manuscript is currently in progress alongside the ongoing study on twisted CNTYs.

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Development of Tensor-Network-based Monte Carlo Methods

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Recently, tensor-network (TN)-based sampling has emerged as a promising alternative to conventional local-update Monte Carlo (MC) methods for frustrated and disordered systems. Whereas earlier TN methods were primarily used as deterministic tools to evaluate partition functions, free energies, and related thermodynamic quantities, more recent work has explored their use for sampling itself, either through conditional-probability-based generation or through collective MC proposals corrected by Metropolis sampling. This approach has already shown promise for random-bond Ising models and has even been extended to three-dimensional spin glasses. At the same time, it has become clear that direct TN-based sampling faces a central limitation: in strongly frustrated systems at low temperatures, the underlying TN contraction can become numerically unstable. Our collaborative work addresses this situation in two complementary directions: one study demonstrates that TN-based sampling can resolve subtle phase-transition structures in a modified spin-glass model [1], while the other proposes a new hybrid framework, tensor-network population annealing (TNPA) [2], specifically designed to overcome the low-temperature instability of existing TN-based samplers.

First, we applied a TN-based hierarchical sampling scheme to a modified Nishimori model on the two-dimensional square lattice [1]. Because the bond variables in this model are correlated, direct sampling is com-

putationally demanding. Our framework enables hierarchical, independent generation of both bond and spin variables, enabling high-precision calculations at large sizes. Using these data, we obtained clear numerical evidence that the ferromagnetic and spin-glass transitions on the Nishimori line are separated, supporting the existence of an intermediate Mattis-like spin-glass phase.

Second, we proposed a new low-temperature sampling method, TNPA [2]. The motivation is the complementary weakness of direct TN-based sampling and conventional population annealing (PA): the former becomes unstable at low temperatures, while the latter requires a long annealing schedule when initialized from the high-temperature limit. TNPA uses TN only for initialization within a reliable temperature range, then uses PA for subsequent low-temperature equilibration, assigning distinct roles to the two methods. The method also introduces an effective-sample-size-based diagnostic that adaptively selects the initialization temperature for each disorder instance. In this sense, TNPA is not just a hybrid of two existing algorithms, but a principled division of work designed to overcome the low-temperature bottleneck of previous TN-based samplers.

Overall, these studies establish TN-based sampling as a practical and promising framework for the numerical study of disordered frustrated systems.

[1] arXiv:2603.18486, [2] arXiv:2604.11155

Generation of spin model with higher-order spin interactions based on machine learning

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Spin textures exhibiting properties fundamentally distinct from conventional ferromagnetic and antiferromagnetic states have attracted significant attention in condensed matter physics. In particular, magnetic skyrmions—topologically nontrivial spin configurations with swirling structures—have emerged as central objects in the study of topological magnetism since their experimental discovery in 2009. While skyrmion crystal phases, characterized by periodic arrangements of such topological objects, have been observed in a wide range of materials, a comprehensive understanding of the microscopic conditions that stabilize these phases—especially the roles of lattice geometry and complex magnetic interactions—remains incomplete. In this context, recent developments in machine learning provide a powerful framework for systematically constructing effective spin models beyond conventional pairwise interactions. In the project 2025-Ca-0003, we have employed machine-learning-based approaches to generate spin Hamiltonians incorporating higher-order spin interactions, aiming to uncover the essential ingredients for stabilizing skyrmion crystal phases under diverse physical conditions. Through extensive numerical simulations, we have identified key mechanisms by which higher-order interactions promote nontrivial spin textures and stabilize skyrmion crystals across different lattice structures. We have also gained key insights into the stabilization mechanisms of topological spin textures through large-scale Monte

Carlo simulations. The main results obtained this year are summarized below.

(i) *Stabilization of skyrmion crystals via higher-order spin interactions and inverse model design:* We have investigated the stabilization mechanisms of topological spin textures by focusing on higher-order spin interactions, particularly four-spin couplings, in frustrated magnetic systems [1]. By developing a theoretical framework that connects real-space four-spin interactions to their effective momentum-space representations, we established an inverse design approach for constructing spin Hamiltonians that realize target multiple- Q states. Using this approach, we successfully designed a minimal model incorporating nearest-neighbor four-spin interactions that stabilizes a skyrmion crystal with a topological number of two per magnetic unit cell even in the absence of an external magnetic field. Large-scale Monte Carlo simulations revealed that such higher-order interactions induce an instability from single- Q spiral states toward multiple- Q superpositions, thereby stabilizing complex spin textures. Furthermore, we demonstrated that the physically relevant ring-exchange interaction naturally generates effective interaction channels favorable for skyrmion formation, leading to the emergence of skyrmion crystal phases and their field-induced transitions. These results provide a unified understanding of how higher-order interactions promote topological magnetic order and offer a systematic pathway for designing spin models hosting complex spin

textures.

(ii) *Finite-temperature stabilization of skyrmion crystals based on momentum-space analysis:* We have investigated the finite-temperature stability of skyrmion crystal phases in frustrated magnetic systems by analyzing the momentum-space exchange interactions of a triangular-lattice Heisenberg model [2]. Through large-scale Monte Carlo simulations, we demonstrated that skyrmion crystals emerge as thermally stabilized multiple- Q states, even when the ground state is a single- Q spiral state. We identified two key factors governing their stability: the sixfold anisotropy of the momentum-space interaction, which acts as a locking potential selecting triple- Q ordering, and the energy of the uniform spin mode, which correlates with the appearance of the skyrmion phase. A larger sixfold anisotropy enhances the stability region of the skyrmion crystal in the temperature-magnetic-field phase diagram, while a sufficiently large uniform-mode contribution is required for its emergence. These results reveal that the stabilization of skyrmion crystals at finite temperatures is driven by an interplay between energetic competition and entropic effects encoded in the momentum-space interaction landscape. Our findings provide a systematic understanding of thermal stabilization mechanisms and offer guiding principles for designing frustrated magnetic systems hosting robust skyrmion phases.

(iii) *Square skyrmion lattice in multiorbital f -electron systems:* We have theoretically investigated the emergence of square skyrmion lattices (S-SkLs) in centrosymmetric tetragonal f -electron systems by incorporating multiorbital effects originating from spin-orbit coupling and crystalline electric fields [3]. Using a mean-field analysis of an effective localized model with two Kramers doublets, we revealed that an S-SkL with skyrmion number of one is stabilized in an intermediate magnetic-

field region when the crystal-field splitting between the doublets is moderate. The phase diagram shows that the S-SkL appears only when multiorbital degrees of freedom are active, while it disappears in the large-splitting limit where the system effectively reduces to a single-orbital model. The S-SkL is characterized by a double- Q magnetic structure with fourfold symmetry and finite scalar chirality, as confirmed by the structure factor and real-space spin configurations. We further identify another multiorbital-induced double- Q state with nonzero scalar chirality at low fields, as well as a variety of competing multiple- Q phases, highlighting the richness of magnetic textures in multiorbital systems. These results demonstrate that multiorbital effects provide a new mechanism for stabilizing skyrmion crystals in centrosymmetric systems, offering a pathway toward realizing S-SkLs in f -electron materials such as Ce-based compounds.

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Dynamical scaling study of three-dimensional $SU(2)$ gauge glass model

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The $SU(2)$ gauge glass (GG) model is a random model that exhibits a ferromagnetic (FM) phase and a spin glass (SG) phase at low temperatures. The Hamiltonian is expressed as

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \text{Tr} \left(\phi_i \omega_{ij} \phi_j^\dagger \right),$$

where a spin variable ϕ_i and a quenched random variable ω_{ij} are $SU(2)$ matrices. The distribution of ω_{ij} is

$$P(\omega_{ij}) \propto \exp(D \text{Tr} \omega_{ij}),$$

where $D = 0$ means the uniform distribution and $D = \infty$ corresponds to the regular case. We apply the dynamical scaling analysis to this model in three dimensions and obtain some locations of critical points and corresponding critical exponents, in order to discuss the critical universality classes of FM and SG transitions.

Like the $\pm J$ Ising model, it possesses gauge symmetry and features the Nishimori line [1]. On the Nishimori line, the exact energy and the upper bound of the specific heat can be obtained analytically, and the relation between FM and SG order parameters, $m = q$, holds. It is also derived that this line passes through a multicritical point (MCP), and the phase boundary at low temperatures is either vertical or reentrant. While such models with gauge symmetry exist for single-component Ising systems and two-component XY systems, they have not yet been identified for three-component Heisenberg systems (though they do exist for Potts systems).

By introducing four real numbers σ_i and $\boldsymbol{\pi}_i = (\pi_{i1}, \pi_{i2}, \pi_{i3})$, the spin variable ϕ_i can be parametrized as

$$\phi_i = \sigma_i I + i \boldsymbol{\tau}_i \cdot \boldsymbol{\pi}_i,$$

where I is the identity matrix and $\boldsymbol{\tau} = (\tau_1, \tau_2, \tau_3)$ are the Pauli matrices. The $SU(2)$ GG model corresponds to a four-component $O(4)$ model in its regular limit

$$\mathcal{H}_0 = -J \sum_{\langle ij \rangle} \text{Tr} \left(\phi_i \phi_j^\dagger \right) = -J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j,$$

where

$$\mathbf{S}_i = (\sigma_i, \pi_{i1}, \pi_{i2}, \pi_{i3})$$

is a unit $O(4)$ vector with $\sigma_i^2 + \pi_{i1}^2 + \pi_{i2}^2 + \pi_{i3}^2 = 1$. Thus the $SU(2)$ GG model can be regarded as an $O(4)$ random system with gauge symmetry [1]. Evaluating the phase diagrams and critical exponents of models with these properties—and understanding the trends in the critical universality of gauge glass models in general—is highly beneficial for gaining a comprehensive overview of random systems as a whole.

At the paramagnetic (PM)-FM boundary, we measured the magnetization relaxation $m(t)$ for $1/D = 0$ (the $O(4)$ model), $1/D = 0.2, 0.5$, and on the Nishimori line ($1/D = T$). Calculations were carried out on a $L = 151$ cubic lattice with the skew boundary condition. We then precisely evaluated the transition temperatures through dynamical scaling analysis using Gaussian process regression (GPR) [2]. At these transition temperatures, the relaxation functions of $m(t)$, the magnetic susceptibility $\chi(t)$, and the temperature derivative of magnetization $\partial m(t)$ were measured with high precision. Calculations were carried out on a $L = 81$ cubic lattice up to 2000 MCS with 10^6 samples. By evaluating the logarithmic derivatives via GPR [3], we determined the thermodynamic critical exponents in the $t \rightarrow \infty$ limit. The results are summarized in Table 1.

Table 1: Results for the FM transition

$1/D$	T_c	ν	z
0	2.137247(3)	0.7465(14)	1.982(1)
0.2	1.78676(7)	0.7476(20)	2.041(1)
0.5	1.26776(4)	0.7482(9)	2.112(1)
T	0.7284(2)	0.987(1)	2.767(1)

Regarding the PM-SG boundary, we measured the relaxation of the SG susceptibility

$$\chi_{\text{SG}}(t) = \frac{1}{N} \left[\sum_{ij} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle^2 \right]$$

for $1/D = \infty$ and $1/D = 2.0$. Calculations were carried out on a $L = 151$ cubic lattice with the skew

boundary condition. Through dynamical scaling analysis using GPR, we estimated the transition temperatures with high accuracy and simultaneously obtained the critical exponents $\gamma_{\text{SG}}/z_{\text{SG}}\nu_{\text{SG}}$ and $z_{\text{SG}}\nu_{\text{SG}}$ [4, 5]. At the determined transition temperatures, we measured the SG correlation function

$$f_{\text{SG}}(r, t) = \frac{1}{N} \left[\sum_i \langle \mathbf{S}_i \cdot \mathbf{S}_{i+r} \rangle^2 \right]$$

and derived the dynamical correlation length $\xi_{\text{SG}}(t)$ at each time step from its dynamical scaling [6, 7]. Calculations were carried out on a $L = 251$ cubic lattice up to 1000 MCS. From the asymptotic behavior of $\xi_{\text{SG}}(t)$, we evaluated the thermodynamic critical exponent z_{SG} . The results are presented in Table 2.

Table 2: Results for the SG transition

$1/D$	T_{SG}	ν_{SG}	z_{SG}
2.0	0.450(2)	1.81(4)	2.93(6)
∞	0.440(1)	1.84(1)	3.01(1)

For the regular case ($1/D = 0$), the transition temperature and critical exponents for the $O(4)$ model are consistent much with those obtained previously [8, 9]. The results in Table 1 suggest that the FM boundary belongs to the same universality class as the regular system, except at the MCP. Since the specific heat exponent α of the regular system is negative, this indicates that the Harris criterion is satisfied. On the other hand, Table 2 shows results that are consistent with the hypothesis that universality also holds for the SG boundary, excluding the MCP. The dynamic critical exponent is shown to increase with increasing randomness, a trend that has also been observed in other gauge glass systems (such as the Ising spin glass). Furthermore, it is evident that the MCP forms its own independent critical universality class.

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Evaluation of Self-Healing Performance and Microscopic Damage in Vitrimers via Molecular Simulations

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We have studied covalent bond healing and microscopic damage accumulation in epoxy vitrimer systems using massive parallel molecular dynamics (MD) simulations. Vitrimers exhibit dynamic covalent bonding associated with disulfide bond (S-S) which enables network rearrangement and self-healing behavior. However, conventional studies have mainly focused on bond exchange reactions, and the direct recombination of broken covalent bonds has not been fully clarified [1].

In this study, we focus on post-scission recombination processes of disulfide bonds and their contribution to network repair. A multi-scale computational framework combining quantum chemical calculations and molecular dynamics (MD) simulations have been employed to elucidate the molecular mechanisms and their impact on macroscopic mechanical properties.

First, quantum chemical calculations based on the GRRM method are performed to explore energetically accessible recombination pathways of sulfur-centered radicals generated by disulfide bond cleavage. As shown in Fig. 1, multiple bonding configurations were identified along the recombination pathway, including

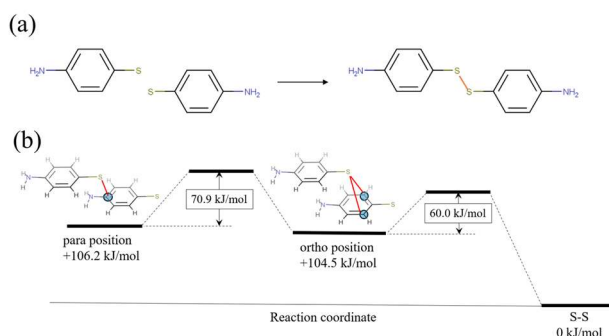


Fig. 1: (a) Recombination reaction of disulfide bonds considered in this study, and (b) Recombination reaction pathway identified by quantum chemical calculations.

transient sulfur-carbon interactions at the ortho and para positions of the benzene ring. These configurations are higher in energy than the fully recombined disulfide bond but remain energetically accessible after bond scission.

Importantly, these intermediate states are not conventional stable bonds but metastable configurations with partial covalent character, which facilitate migration of radicals prior to recombination. This result indicates that bond healing proceeds not only through direct S-S recombination but also through intermediate states involving aromatic interactions. This finding provides a new perspective on vitrimer healing mechanisms, highlighting the importance of post-scission pathways distinct from conventional bond exchange reactions.

Second, large-scale MD simulations are

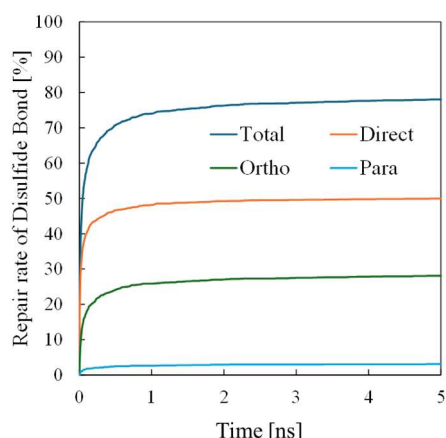


Fig. 2: Time evolutions of the repair rate of disulfide bonds during the damage recovery simulation.

conducted to evaluate the deformation behavior and healing processes of a cross-linked epoxy vitrimer network (~27,000 atoms). The simulation workflow consists of:

1. Construction of a cross-linked network
2. Tensile deformation with bond scission
3. Damage recovery via bond recombination
4. Re-evaluation of mechanical properties

During deformation, disulfide bonds are found to preferentially break compared with other covalent bonds. This selective bond scission suppresses catastrophic failure and distributes damage throughout the network.

The self-healing process for the crosslinked network is simulated by introducing our finding recombination reactions based on quantum chemical results. As shown in Fig. 2, approximately 78% of broken disulfide bonds were recovered within several nanoseconds. The healing process consists of two main pathways, direct sulfur–sulfur recombination (~64%) and Ortho-mediated recombination via transient S–C bonding (~36%). This clearly

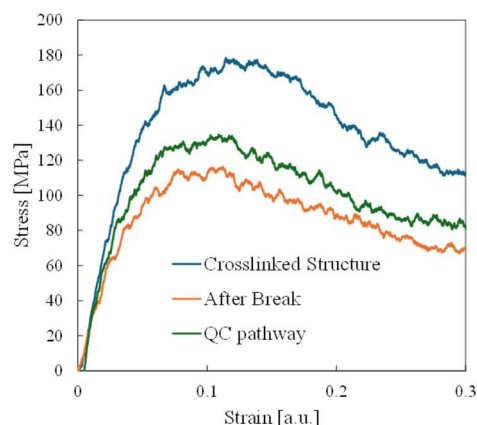


Fig. 3: Stress–strain curves obtained from uniaxial tensile deformation of three different network.

demonstrates that the quantum chemically identified recombination pathway significantly contributes to network repair.

The effect of bond healing on macroscopic mechanical properties is evaluated by tensile simulations. As shown in Fig. 3, the stress–strain responses reveal healed network shows partial recovery. Both Young's modulus and tensile strength are restored to an intermediate level after healing, demonstrating that microscopic bond recombination directly contributes to macroscopic property recovery.

In conclusion, we have investigated covalent bond healing in epoxy vitrimer systems using QM calculations and MD simulations. The results showed that disulfide bonds preferentially break and are partially reformed, leading to recovery of mechanical properties.

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Coherent current generation in graphene driven by structured light fields

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We have studied coherent electronic and spin-related responses in crystalline solids driven by intense light fields using large-scale time-dependent simulations. The original motivation of this project was to clarify the microscopic mechanism of THz-induced spin magnetization accumulation in semiconductors, where coherent interband polarization and spin-orbit coupling play essential roles. During this year, we focused on developing and testing a computational framework for light-induced coherent currents and magnetic responses in a prototype two-dimensional material. In particular, we investigated graphene driven by spatially structured Laguerre-Gaussian beams, whose intensity and phase vary in real space and whose polarization state can be controlled.

The time-dependent electronic dynamics were calculated in momentum space by propagating the quantum states under pulsed optical fields [1–4]. The photoinduced current was then evaluated from the time-evolved states, and its angular dependence was decomposed into winding-number components. This analysis enabled us to identify how the orbital angular momentum and polarization helicity of light select different dc current channels. Since the calculations require dense sampling of the

Brillouin zone, time propagation for many optical parameters, and repeated simulations for different angular positions and beam profiles, the ISSP supercomputer system was essential for carrying out this study.

The numerical code was parallelized mainly over momentum-space grid points and optical/angular parameters using MPI. We further optimized the calculations by precomputing field-dependent and geometrical factors, reducing redundant evaluations inside the time-evolution loop, and organizing the output files so that the winding-number analysis could be performed without repeating the computationally expensive real-time propagation. These improvements enabled systematic parameter scans over the optical angular momentum, polarization helicity, field strength, pulse duration, and radial position of the structured light field.

As a result, we obtained winding-number-resolved spectra of the dc current induced by structured light in graphene, with separate analysis of local and gradient-induced current components. Figure 1 shows representative spectra for optical angular momenta $l = 1$ and $l = 2$. The dominant winding channels are switched by changing the polarization helicity

and optical angular momentum. In addition, the selected channels differ between the local and gradient-induced current components, indicating that the spatial structure of the light field provides a way to distinguish different microscopic current-generation mechanisms. In particular, the selective appearance of the $m = 0$ component is important because it is directly connected to circulating photocurrents and the resulting magnetic response. These results provide a basis for evaluating light-induced magnetic responses, thereby connecting the present calculations to the original goal of controlling spin and magnetic responses in solids. Although the full three-dimensional

simulation of spin magnetization accumulation in GaAs remains a challenging next step, the present calculations established an important numerical and physical foundation for future studies.

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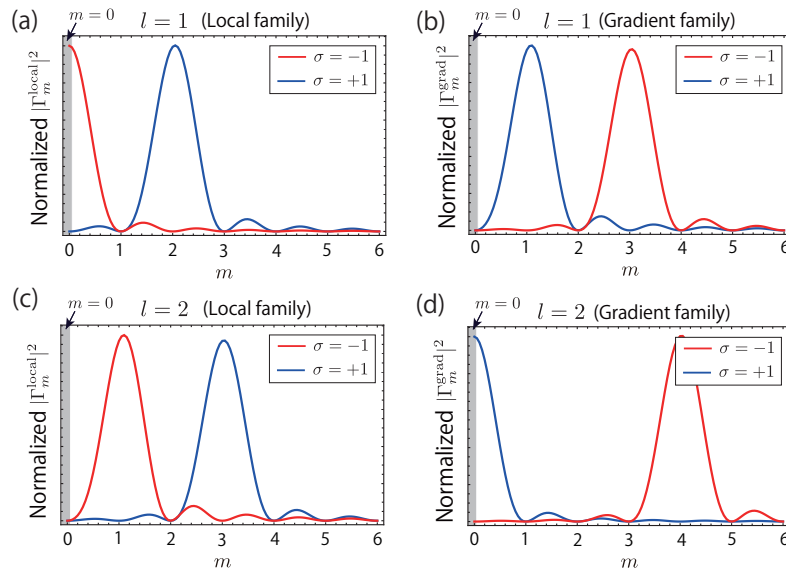


Fig. 1: Winding-number-resolved spectra of dc currents induced in graphene by Laguerre-Gaussian beams. Panels (a,b) and (c,d) show the results for optical angular momenta $l = 1$ and $l = 2$, respectively. Local and gradient-induced current components are shown separately. Red and blue curves represent opposite polarization helicities, $\sigma = -1$ and $\sigma = +1$. The helicity-dependent peak positions demonstrate selective activation of different winding-number channels. The arrows indicate the $m = 0$ channel, which is related to circulating photocurrents and magnetic responses.

Simulated tempering simulations of model silica glasses

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Both experiments and computer simulations of glass-forming liquids experience a drastic growth of the relaxation time at low temperatures. Only a few percent change in temperature of glasses can result in decades slower dynamics, whereas its static structures remain disordered. Understanding the physical origin of the slow glassy dynamics has been a central problem of the glass physics, and accessing equilibrium glassy states at low temperature is challenging.

In the last decade, the Swap Monte Carlo algorithm has revolutionized the computer simulations of glasses [1, 2]. The algorithm simply attempts to swap particle diameters of randomly chosen pairs of particles. Despite its simplicity, this algorithm can reduce the timescale of tailored polydisperse models at low temperatures by many orders of magnitude, thereby allowing us to access very stable glassy states and to study their thermodynamic and mechanical properties in detail. However, when applied to binary systems, such as silica glasses, it cannot accelerate the dynamics much, as swapping different types of particles is barely accepted at low temperature. Different strategies are thus needed to sample stable glass configurations of such systems.

Here, we apply simulated tempering (ST) [4] to a model silica glass in three dimensions [3] and test if it can efficiently equilibrate the system at very low temperatures. In ST simulations, we dynamically change temperature (or

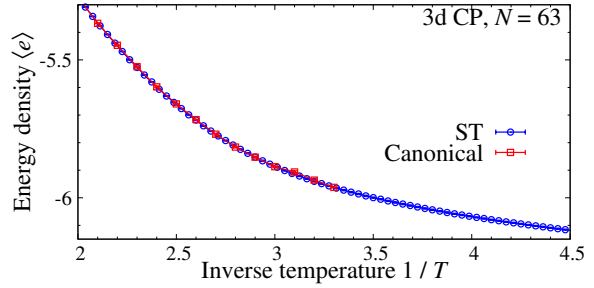


Figure 1: Mean energy density $\langle e \rangle$ obtained with canonical and ST simulations, represented by red square and blue circular points, respectively.

any other intensive control parameters) of the system with maintaining equilibrium at any time, in addition to updating the microscopic degrees of freedom as usual. The range of temperature needs to be set so that the system in the high-temperature regime can decorrelate rapidly, and that particle configurations at low temperatures are statistically independent after each round trip in the temperature space. Unlike the exchange Monte Carlo (also known as parallel tempering) [5], unfortunately, ST needs careful tuning of parameters to have the algorithm reach the whole temperature space. We have iteratively adjusted the parameters with extensive parallelization of preliminary ST simulations on the ISSP Supercomputer System B, which has accelerated the process by a factor of ≈ 50 .

We show the energy density $\langle e \rangle$ of the model with the number of particles $N = 63$. Canonical simulations (i.e., local Monte Carlo simula-

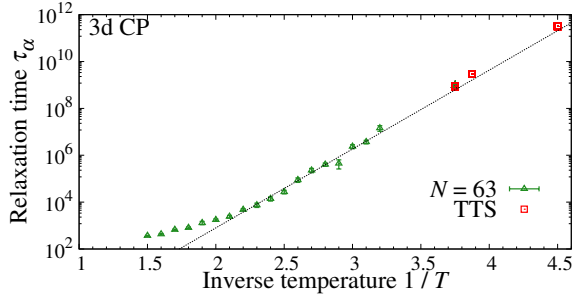


Figure 2: Structural relaxation time τ_α as a function of inverse temperature β of the model with $N = 63$. Green triangular and red square points represent τ_α measured with initial configurations generated by the local Monte Carlo dynamics and ST simulations, respectively. For the latter case, τ_α is estimated using the time-temperature superposition (TTS) assumption.

tions without the tempering process) and ST ones yield results consistent with each other, confirming the correctness of the ST algorithm. The local Monte Carlo as well as molecular dynamics can reach up to $\beta \approx 3.3$ for this model [3], as the dynamics in this temperature regime is so slow – the structural relaxation time τ_α , which is defined as the timescale of the time correlation of particle positions, grows exponentially with β and exceeds 10^8 at $\beta \approx 3.5$, see Fig. 2. On the other hand, ST can reach equilibrium states at much lower temperatures, e.g., $\beta = 4.5$, within 10^8 Monte Carlo sweeps per particle, therefore accelerating the dynamics by several orders of magnitude. To verify configurations from ST runs at that low temperature are compatible with other equilibrium data, we study the dynamics of the local Monte Carlo dynamics starting from configurations obtained by ST runs. Since the dynamics there is so slow that the time correlation does not decay to a small value within simulation times, we estimate τ_α with the time-temperature superposition assumption [6]. We find τ_α measured in this protocol is indeed consistent with an Arrhenius curve for τ_α at higher temperatures (see Fig. 2). In future work, we

will apply the algorithm to larger system sizes and more realistic models to establish ST as a efficient tool to access stable glassy states.

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Defect structures and their transport properties in thermoelectric chalcogenides

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In this project, we investigated nanoscale thermal transport at grain boundaries (GBs) in PbTe, a representative thermoelectric material, by combining machine-learning interatomic potentials with large-scale perturbed molecular dynamics (MD) simulations. The main objective was to clarify how GB atomic structures affect lattice thermal conductivity and to establish a basis for improving the thermoelectric performance through defect engineering.

The most intensive use of the ISSP supercomputer resources was devoted to large-scale atomistic simulations based on a neural-network potential (NNP). Direct evaluation of thermal transport for GBs by DFT is prohibitively expensive, because both structural optimization and finite-temperature transport calculations require large supercells and long simulation times. To overcome this difficulty, we employed an NNP trained on DFT data for bulk, point defects, surfaces, and GB structures [1]. This strategy retained high accuracy for GB energetics and atomic forces while reducing the computational cost by several orders of magnitude compared with direct DFT calculations. As a result, it became possible to perform systematic simulations for 24 symmetric tilt GBs in PbTe, including both [001] and $[1\bar{1}0]$ rotation-axis systems [2].

The largest share of the supercomputer time was spent on perturbed MD calculations of

lattice thermal conductivity. For each lowest-energy GB structure with different misorientations, we constructed supercells containing two equivalent GBs, with lengths of approximately 100 Å along the GB-normal direction and more than 45 Å along the in-plane directions. Lattice thermal conductivity was evaluated not only normal to the GB plane but also along the two GB-parallel directions. Because each conductivity calculation requires long-time averaging under finite perturbation within the linear-response regime, and because this procedure was repeated for many GB models and multiple heat-flux directions, the total computational demand was substantial. In addition, atom-resolved and wave-decomposed analyses were carried out from the same PMD framework to identify the microscopic origin of the anisotropic thermal transport.

Using this computational framework, we showed that the GB thermal resistance in PbTe varies by as much as a factor of seven depending on GB structure (Fig. 1). Along the direction normal to the GB plane, the thermal conductivity tends to decrease as the coordination-number change at the GB increases. In contrast, along the GB-parallel directions, the thermal conductivity is influenced more strongly by bond-length distortion and crystallographic orientation. We further found that the influence of GBs on heat transport parallel to the boundary extends over

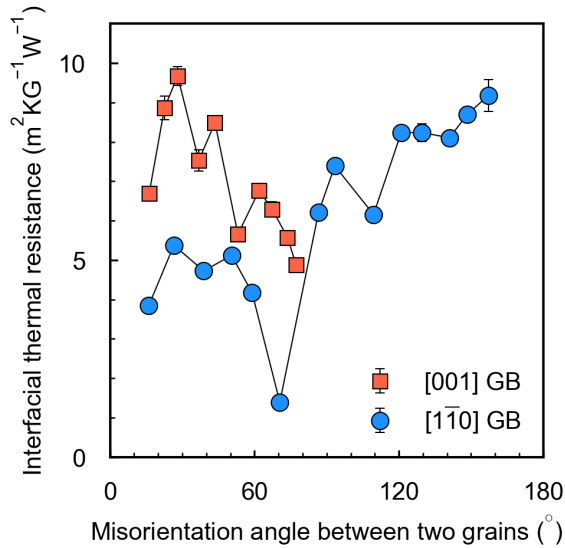


Figure 1: Interfacial thermal resistance of PbTe GBs as a function of GB misorientation angle. The results for GBs with $[001]$ and $[1\bar{1}0]$ rotation axes are shown. Adapted from Ref. [2] under CC BY 3.0.

roughly 10 nm from the GB plane, indicating that in-plane transport suppression is also non-negligible in nanocrystalline PbTe.

Overall, this project demonstrated that NNP-based atomistic simulation is a powerful approach for quantitatively analyzing defect-dependent thermal transport in thermoelectric materials. The ISSP supercomputer played a central role by enabling extensive NNP-MD sampling, systematic GB-structure searches, and repeated PMD calculations over many large supercells. These computations yielded a microscopic and quantitative picture of how structurally diverse GBs control lattice thermal conduction in PbTe.

In addition to these results, several tens of further calculations of GB thermal conductivity and electronic transport have been carried out. These large-scale simulations are steadily providing new insights toward elucidating the structure–property relationships in GBs and providing a basis for future microstructure

design of high-performance thermoelectric materials.

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Molecular Analysis of Surface Tension Changes in Mixed Ionic Liquids via Large-Scale MD Simulation on ISSP Supercomputer System

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Ionic liquids (ILs) are promising materials for CO₂ separation membranes owing to their negligible volatility and high gas solubility [1]. Precise control of surface tension is critical for stable IL retention within support membranes. Although mixing multiple ILs is an effective strategy to tune physicochemical properties [2], the surface tension of mixed ILs deviates from ideal mixing [3], and the underlying molecular mechanism remains poorly understood. In this study, large-scale MD simulations were performed on the ISSP supercomputer (ohtaka) to reproduce the gas–liquid interface of mixed imidazolium-based ILs ([C_nmim][NTf₂], $n = 2, 4$) and to elucidate the molecular origin of the nonlinear surface tension change upon mixing.

A total of 4096 ion pairs (~57,000 atoms) were placed in a simulation box ($\sim 200 \times 120 \times 120$ Å³) to construct a slab model. MD simulations were performed using LAMMPS [4] with the OPLS-AA-based force field [5–7], with MPI parallelization across 128 cores per job on ohtaka (~2,000 CPU-core hours per system). Surface tension was evaluated via the Kirkwood–Buff mechanical route [8], and local

stress distributions were analyzed using the volume averaging method (VAM) [9] at 1 Å resolution.

Number density profiles (Fig. 1) show that the outermost layer is enriched in nonpolar moieties (alkyl chains) in all systems. In the equimolar mixture, C₄mim is markedly enriched in the outermost layer, reflecting selective surface adsorption of the longer alkyl chain. The polar layer in the mixture (12.0 Å) is thicker than in single-component systems (7.5 Å), due to a sublayer structure from the coexistence of two cation species.

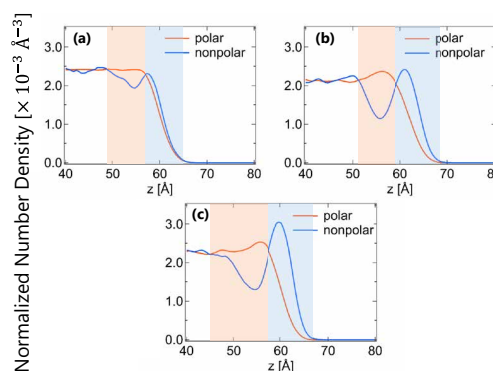


Fig. 1: Normalized number densities of polar (red) and non-polar (blue) moieties across the interface for (a) [C₂mim][NTf₂], (b) [C₄mim][NTf₂], and (c) the mixture.

Decomposition of the local stress tensor anisotropy by interaction type (Fig. 2) revealed that the majority of net surface tension originates in the polar layer in all systems; intermolecular interactions (Coulomb and LJ) produce large positive peaks near the interface, while intramolecular interactions (bond, angle) provide partially canceling contributions. The calculated surface tensions were 44.8 mN/m ($C_2\text{mim}$), 31.4 mN/m ($C_4\text{mim}$), and 35.0 mN/m (mixture), with a deviation of -3.1 mN/m from ideal mixing (Fig. 3). This deviation is dominated by the Coulomb term (-23.9 mN/m), indicating that coexistence of two cation species in the polar layer alters the local electrostatic environment, a finding enabled by high-resolution local stress analysis on the ISSP supercomputer.

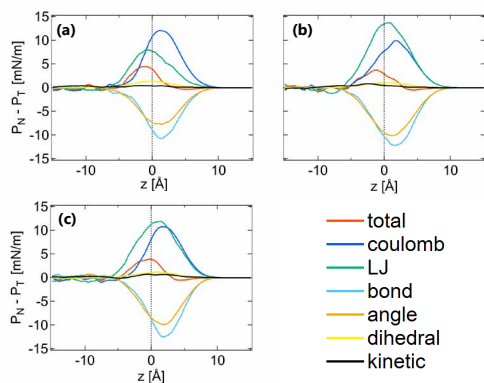


Fig. 2: Surface tension contributions decomposed by interaction type for (a) $[C_2\text{mim}][\text{NTf}_2]$, (b) $[C_4\text{mim}][\text{NTf}_2]$, and (c) the mixture.

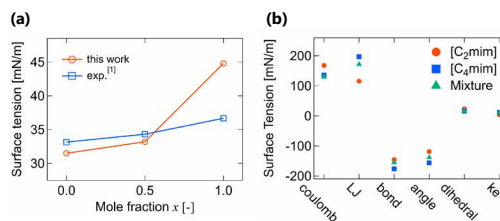


Fig. 3: (a) Composition dependence of surface tension. (b) Decomposition into interaction components for $[C_2\text{mim}][\text{NTf}_2]$ (red), $[C_4\text{mim}][\text{NTf}_2]$ (blue), and the mixture (green).

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Quantum emulator using GPU toward fault-tolerant quantum computing for reacting flow analysis

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This study presents a GPU-based emulator for Quantum Phase Estimation (QPE) designed for practical quantum applications in science and engineering. As shown in Figure 1, the QPE circuit is built from measurement qubits, controlled powers of the target unitary, and an inverse quantum Fourier transform, providing the basic structure used throughout the implementation. The emulator was developed with NVIDIA cuQuantum and CUDA, with HDF5-based input and output to make preprocessing and postprocessing straightforward. It was designed to exploit GPU resources aggressively, especially VRAM, so that larger and faster simulations could be achieved.

The implementation was validated using both analytically constructed test cases and random unitary matrices. Benchmark results

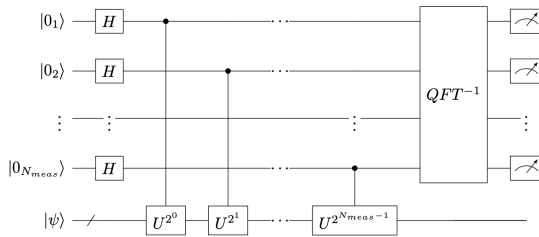


Figure 2 Quantum circuit of quantum phase estimation.

showed that computational cost rises rapidly with total qubit count, while higher-end GPUs provide clear speed advantages. At the same time, the error in estimated eigenphases decreased exponentially as the number of measurement qubits increased. This trend is clearly illustrated in Figure 2, which confirms that adding measurement qubits systematically improves numerical precision. Overall, the work establishes a practical platform for mid-scale quantum emulation and provides a useful computational basis for future applications of quantum algorithms such as QPE and HHL

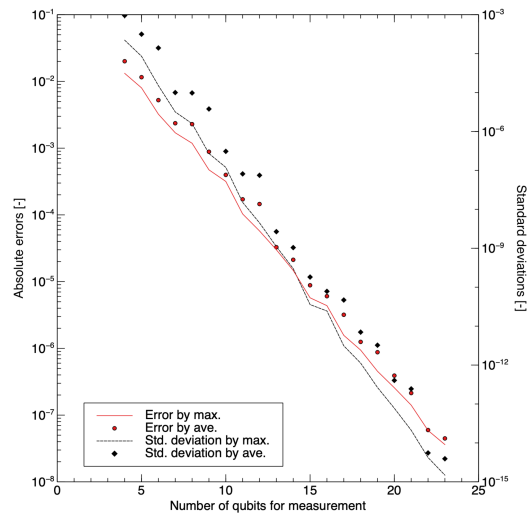


Figure 1 Numerical precision vs the number of qubits for measurement bit.

Theoretical and Experimental Study on Ambipolar Transport and Conduction Path Control in Nickel Dithiolene Complexes

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Molecular organic semiconductors are a class of materials characterized by their flexibility, high structural designability, and the solution-processability inherent to molecular systems. While p-type and n-type unipolar semiconductors with high mobility have already been commercialized, ambipolar semiconductors—which switch between p-type and n-type operation via the application of a gate potential—remain in the developmental stage. The realization of ambipolar behavior requires not only high solubility and highly ordered crystallinity on substrates but also high-dimensional electronic structures that stabilize conduction paths, alongside meeting stringent requirements for the electronic state in the stacked arrangement.

Focusing on these electronic requirements, we investigated nickel dithiolene complexes as d/π -conjugated molecules, which offer high structural designability via side chains and fine-tunability of solubility. These complexes functioned as exceptionally well-balanced ambipolar semiconductors, exhibiting solution-processability, high crystallinity, a two-dimensional (2D) electronic structure derived

from their stacked morphology, and high atmospheric stability [1].

Carrier transport in these materials is governed by HOMO-derived bands for holes and LUMO-derived bands for electrons, originating from their respective molecular orbital interactions. Electronic structure analysis performed using theoretical calculations predicted that within the 2D plane, the HOMO-derived band is anisotropic, whereas the LUMO-derived band is isotropic. This finding implies that the conduction paths for holes and electrons are distinct; more specifically, the direction of carrier flow can be switched depending on the applied potential.

In this study, aiming to manifest this unique functionality, we optimized the solution-processing methods and successfully fabricated single-crystal thin films with large domain sizes of 500 μm^2 . This achievement allowed us to experimentally validate the theoretical predictions. The experimental results showed excellent agreement with the simulations, demonstrating for the first time that carrier-dependent transport paths can be switched by the gate potential [2]. Furthermore, we have

expanded this research to the observation of magnetic anisotropy in aqueous environments [3] and the development of pure π -conjugated systems [4].

This research was conducted during my appointment as an Assistant Professor at the University of Tokyo. The work was performed in collaboration with Professor Mori, members of the Mori Laboratory, and numerous other partners. I would like to express my sincere gratitude for their invaluable support and contributions.

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Numerical study on low-energy states of quantum spin systems

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It is well known that researchers encounter many-body problems in condensed matter physics that make it difficult to accurately estimate physical quantities. The problem of quantum spin systems is a typical one. Numerical approaches have been widely and effectively utilised in the study of quantum spin systems. Computational studies have provided valuable information about the target systems.

Three methods have been successfully employed in the computational studies of quantum spin systems. The numerical diagonalization method is the standard, traditional approach. The second approach is based on a quantum Monte Carlo (QMC) simulation. The third approach is the density matrix renormalization group (DMRG) method. Each of these methods has its own advantages and disadvantages. Regardless of their spatial dimensions, QMC simulations can handle significantly larger systems. However, this approach encounters the negative sign problem when attempting to accurately evaluate physical quantities in frustrated systems. The DMRG method is useful when its spatial dimension is one, regardless of whether or not the target system has frustration. This method is still being developed for cases where the spatial dimension is more than one. The numerical diagonalization method can be used in various systems, no matter what the spatial dimension is or if there are any frustrations. However, this method is only effective for very small systems. To overcome the numerical diagonaliza-

tion method's drawback, we developed a parallel code based on the Lanczos diagonalization method[1]. Using this code, we can treat various large systems that have not yet been treated. In this project, we primarily use this method to analyze various quantum spin systems.

In 2025, this project reported our achievement concerning the spin- S Heisenberg anti-ferromagnet on the orthogonal dimer lattice for $S = 2$ [2] in addition to our previous studies of spin-1/2, 1, and 3/2 cases[4, 3]. In this study, we successfully carried out Lanczos diagonalizations of this system 16 and 20 sites for $S = 2$ case. It is for the first time that within Lanczos-diagonalization studies, numerical results of this model had been presented for $S = 2$ case to the best of our knowledge. We clarified the change of the behavior of this model when the ratio of two interaction amplitudes denoted by $r = J_2/J_1$, where J_1 denotes the amplitude of the Heisenberg interaction at the orthogonal dimer and J_2 denotes the amplitude of interaction forming the square lattice. Consequently, we successfully captured the edge of the exact-dimer phase. At the same time, we also detected the edge of the Néel-ordered phase at a different r from the edge of the exact-dimer phase. We confirmed that differences between systems of the 16 and 20 sites are small in our results with respect to the values of r corresponding each of the edges. Our results strongly suggest that the existence of an intermediate phase between both the edges

irrespective of spin- S up to $S = 2$. Combining the results with previous ones, we successfully clarify the systematic S -dependence of the edges of the two phases. The project also investigated the Haldane gap issue in the case of $S = 7$ [5] and successfully provide a numerical estimate for the gap. Our studies contribute greatly to our deeper understanding of quantum magnetism. Further investigations would shed light on the nontrivial quantum effects in these systems.

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The physical picture of Johari-Goldstein relaxation in metallic glasses

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Johari–Goldstein (JG) relaxation, often referred to as slow β relaxation, is a ubiquitous feature of supercooled liquids and glasses and plays a key role in determining material properties such as impact strength, particularly below the glass transition temperature. Despite its importance, the microscopic origin of JG relaxation remains poorly understood, largely due to the difficulty of probing this process experimentally and capturing it accurately in simulations.

In this study, we investigate the relaxation dynamics and mechanical response of a ZrCuAl metallic glass using molecular dynamics simulations with LAMMPS. Cyclic shear deformation is applied, and the loss modulus is evaluated as a function of temperature for systems with different structural stability. We find that, at low temperatures, the loss modulus becomes negligible as the glass becomes more stable. Consequently, the Johari–Goldstein

secondary relaxation is suppressed in highly stable glasses, suggesting that the localized atomic rearrangements responsible for this process are hindered by enhanced stability. We further examine the stress–strain response at zero temperature under applied strain. Two structures are considered: glassy and crystalline configurations of the same ZrCuAl composition, both initially equilibrated at 300 K. The stress–strain curves exhibit clear differences. The glassy system shows a pronounced stress peak, indicative of brittle behavior, whereas the crystalline system exhibits a smoother deformation response. These results highlight the correlation between structural stability, relaxation dynamics, and mechanical properties in metallic glasses.

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Stress propagation in colloidal gels

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This study investigates the mechanical response and yielding behavior of aerogels under isotropic expansion using coarse-grained simulations. Aerogels exhibit linear elastic behavior at small strains, followed by sudden yielding at a critical strain ($\epsilon \approx 0.18$), accompanied by bond rupture and plastic deformation.

The deformation is highly heterogeneous and hierarchical. At small length scales, particles move cooperatively within structurally defined regions, while at larger scales, deformation is dominated by transverse, vortex-like nonaffine displacements. A characteristic length scale separates these regimes and reflects the underlying structural heterogeneity of the gel network.

Mechanical properties are strongly controlled by the bond-creation probability p_{bond} , which determines the network structure. Lower p_{bond} leads to more branched and locally dense structures with higher stiffness but reduced durability, whereas higher p_{bond} results in softer yet more robust networks. This establishes a clear trade-off between bulk modulus and yielding strain.

To understand stress transmission, the study introduces the concept of stretched and directed paths (strDPs), which represent locally stiff regions that carry stress across the system. During deformation, these paths elongate through bond alignment and eventually form system-spanning structures. Yielding occurs when the extension of these paths reaches a limit, leading to mechanical saturation beyond which further deformation induces bond breakage rather than additional structural rearrangement.

Overall, the results provide a unified framework linking microscopic structural organization, cooperative dynamics, and macroscopic mechanical response, offering insights for designing aerogels with tailored stiffness, flexibility, and durability.

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Ground state phase diagram and finite- T Study of Sr_2IrO_4

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Competing interactions in quantum magnets can suppress conventional dipolar magnetic order and stabilize phases characterized by higher-rank spin correlations. A paradigmatic example is a quantum spin nematic (QSN), the quantum magnetic analogue of a liquid crystal, in which spin-rotational symmetry is broken while time-reversal symmetry remains intact. Because QSN order does not carry a static magnetic dipole moment, it is difficult to detect with standard linear-response probes and, thus, can be classified as *hidden order*. In spin-1/2 systems, these higher-rank spin correlations can only emerge from an intricate interplay of the individual spins forming quadrupoles (n-type nematic) [1] or vector-chiral moments (p-type nematic) [2] on bonds.

This makes the recent observation of quadrupolar signatures in the $J_{\text{eff}} = 1/2$ spin-orbit-coupled Mott insulator Sr_2IrO_4 particularly striking [3]. Sr_2IrO_4 is a square-lattice antiferromagnet with well-established canted Néel order, where spin-orbit coupling-induced Dzyaloshinskii-Moriya interactions (DMI) naturally generate vector-chiral bond correlations, yet do not by themselves explain symmetric bond-quadrupolar order. The reported coexistence of dipolar magnetism and QSN-like quadrupolar order therefore poses a question: *why should a spin nematic appear in an antiferromagnetic $J_{\text{eff}} = 1/2$ material, far from the conventional spin-1 or frustrated-ferromagnet settings?*

We have identified a possible resolution based on the algebra of spin-1/2 bond operators [5]. The key point is that antisymmetric vector-chiral bilinears and symmetric quadrupolar bilinears are not independent: the anticommutator of two distinct vector-chiral components on the same bond generates an off-diagonal bond quadrupole. Using a minimal model of Sr_2IrO_4 [4],

$$\begin{aligned} \mathcal{H} = & \sum_{\langle ij \rangle_1} [J_1 \mathbf{S}_i \cdot \mathbf{S}_j + D^z (S_i^x S_j^y - S_i^y S_j^x) \\ & + \Gamma_2 (S_i^x S_j^x - S_i^y S_j^y)] + \sum_{\langle ij \rangle_2} J_2 \mathbf{S}_i \cdot \mathbf{S}_j \\ & + \sum_{\langle ijkl \rangle} J_c [(\mathbf{S}_i \cdot \mathbf{S}_j)(\mathbf{S}_k \cdot \mathbf{S}_l) \\ & + (\mathbf{S}_j \cdot \mathbf{S}_k)(\mathbf{S}_l \cdot \mathbf{S}_i) - (\mathbf{S}_i \cdot \mathbf{S}_k)(\mathbf{S}_j \cdot \mathbf{S}_l)] , \end{aligned} \quad (1)$$

incorporating out-of-plane DMI D^z , Γ_2 due to orthorhombic distortions, and cyclic ring exchange J_c around a square, we identify a spin-nematic phase $VC+AFQ$ illustrating this mechanism [5].

We map out the ground-state phase diagram as a function of the second-neighbor exchange J_2 and cyclic ring exchange J_c at fixed $D_z/J_1 = 0.25$ and $\Gamma_2/J_1 = 0.1$. Besides conventional dipolar phases, including canted Néel, stripe, and four-sublattice antiferromagnetic order, we find an extended $VC+AFQ$ region with finite vector-chiral and antiferro-quadrupolar bond moments but no dipolar long-range order. Most importantly in the context of Sr_2IrO_4 , this spin-nematic phase borders the canted Néel phase through a narrow

coexistence regime in which dipolar, vector-chiral, and quadrupolar moments are simultaneously present. This provides a natural route to the experimentally observed coexistence of canted antiferromagnetism and quadrupolar order.

We further investigate the thermodynamics of these orders using TPQ-MPS simulations. The specific heat shows a broad high-temperature feature associated with the buildup of short-range antiferromagnetic correlations and DMI-induced vector chirality. At lower temperature, the vector-chiral and quadrupolar structure factors grow strongly, followed closely by the onset of canted Néel correlations. This sequence suggests a narrow temperature window in which spin-nematic correlations develop before dipolar magnetic order becomes dominant, consistent with the experimental indication of quadrupolar order appearing above or together with the magnetic transition in Sr_2IrO_4 .

This work has relied heavily on the open source MPS and DMRG package *TenPy* [8] providing parallelization of matrix operations within a single node through optimized LAPACK and BLAS packages.

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Realistic finite-temperature simulations and application to giant magnetocaloric effects with charge–spin–lattice coupling

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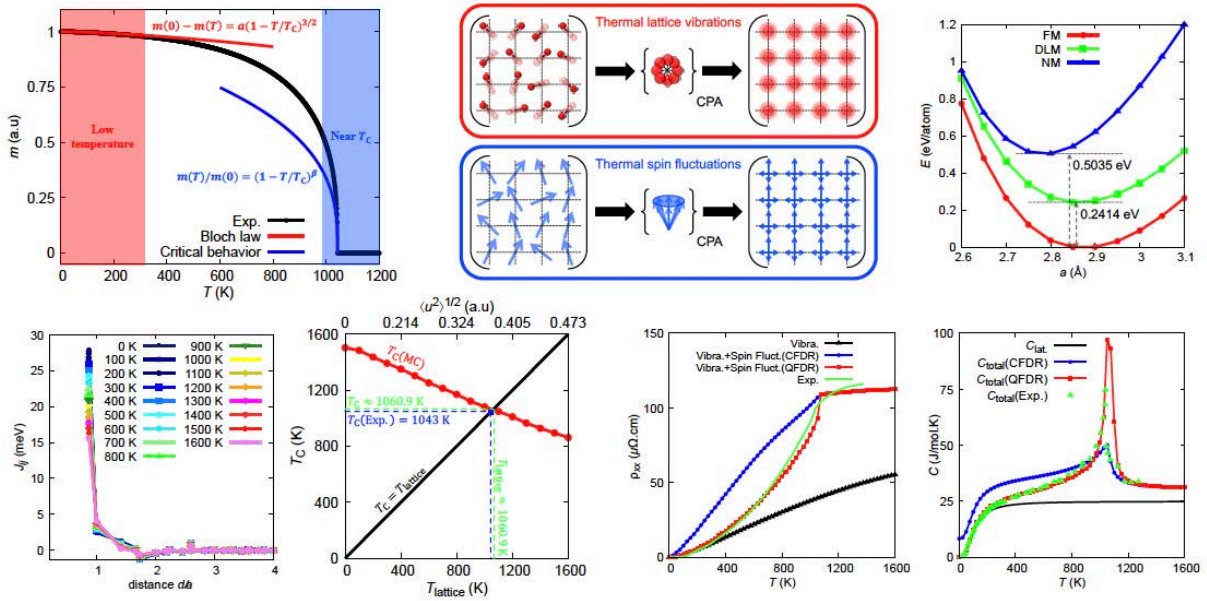


Figure 1: Realistic finite-temperature simulations for magnetic properties of bcc Fe.

Accurate prediction of magnetic properties at finite temperatures is essential for designing functional materials. Conventional simulations based on the classical Heisenberg model fail to reproduce experimental spontaneous magnetization, particularly at low and intermediate temperatures, due to the neglect of the quantization effect of spin. In this work, we developed a realistic finite-temperature simulation framework by combining first-principles calculations with Monte Carlo simulations, including both thermal lattice vibration and spin fluctuation effects[1], as shown in Fig. 1. The magnetic exchange coupling constants J_{ij} are evaluated at finite temperatures with lattice vibration effect. A quantum fluctuation–dissipation relations (QFDR) are introduced to describe thermal energy as magnon excitations using Bose–Einstein statistics.

The developed method significantly improves the temperature dependence of spontaneous magnetization and Curie temperature compared to conventional approaches. The inclusion of thermal lattice vibration reduces the exchange interactions, while quantum spin fluctuations

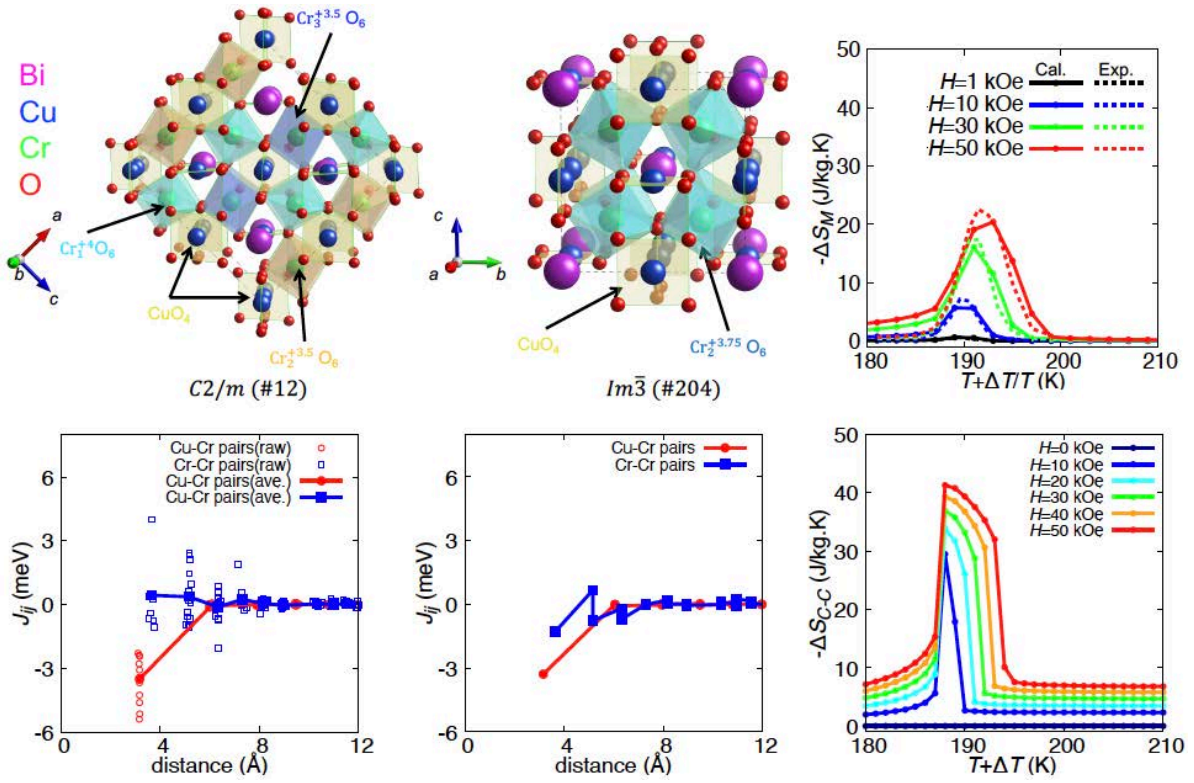


Figure 2: Giant magnetocaloric effect in $\text{BiCu}_3\text{Cr}_4\text{O}_{12}$ with charge–spin–lattice coupling.

correct the low-temperature behavior. This framework enables accurate prediction of magnetic and transport properties at finite temperatures[1].

Based on this method, we further investigated the giant magnetocaloric effect (MCE) in $\text{BiCu}_3\text{Cr}_4\text{O}_{12}$, where strong charge–spin–lattice coupling plays a key role[2]. This material exhibits a first-order magnetostructural transition between $C2/m$ and $Im\bar{3}$ phases, accompanied by charge disproportionation, as shown in Fig. 2. To describe this behavior, we employed a mixed-phase model combining magnetic and lattice contributions, and evaluated the entropy change using both Maxwell relations and the Clausius–Clapeyron equation.

The giant MCE originates from the strong interplay between charge, spin, and lattice degrees of freedom. In contrast to conventional systems, the entropy change includes significant lattice and electronic contributions in addition to the magnetic component. This coupling enhances the total entropy change through a first-order phase transition, providing a new mechanism for large MCE.

In summary, we developed a realistic finite-temperature simulation framework and demonstrated its application to magnetocaloric materials. The results reveal that multi-physics coupling is essential for accurately describing and enhancing magnetocaloric effects, providing a guideline for designing next-generation energy-efficient cooling materials.

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Multiphase-Reactive Simulations of Aluminum Particle Combustion with Detailed Kinetics and Interfacial Phase Change

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In recent years, aluminum (Al) has attracted considerable attention as a potential carbon-free fuel for thermal energy systems [1]. Recently, extensive efforts have been made to develop Al combustion models. Most research has incorporated detailed chemical kinetics for Al oxidation, while treating the complex phase-change process with analytic approaches and relying on restrictive assumptions. These simplifications significantly limit their applicability to practical combustion environments.

To address these limitations, we developed an interface-resolved multiphase CFD model for Al particle combustion based on the Volume-of-Fluid (VOF) method, to fully resolve mass and heat transfer processes at the liquid-gas interface, to capture droplet deformation and the complex physicochemical phenomena that arise during combustion, and to reveal both species consumption/generation behavior and global combustion characteristics.

The model is validated by comparing the predicted particle/droplet diameter evolution under pure evaporation conditions with

experimental data. Here, we simulate the microgravity evaporation of isolated *n*-heptane droplets in nitrogen and compare the numerical results with experimental data by Nomura et al. [2]. As shown in Fig. 1, the squared droplet diameter exhibits an approximately linear decay, consistent with the classical d^2 -law. Comparisons between our numerical predictions and experimental data show good agreement, especially at higher temperatures. As the droplet diameter decreases, the discrepancy between predictions and measurements becomes non-negligible, which can be attributed to the neglect of gravity effects.

The combustion of a 93 μm Al particle under the conditions $X_{\text{O}_2} = 0.21$, $X_{\text{N}_2} = 0.79$, $T = 300$ K is simulated. To initiate ignition, an external volumetric heat source term $\mathbf{q}_{\text{ext}} = 100$ $\text{MW/m}^3/\text{K}$ is applied uniformly within the Al particle. This source remains active until the average particle temperature reaches $T_0 = 2327$ K. Under this configuration, ignition is achieved within approximately 0.013 ms.

Figure 2 shows the evolution of the radial temperature profiles. After ignition, the

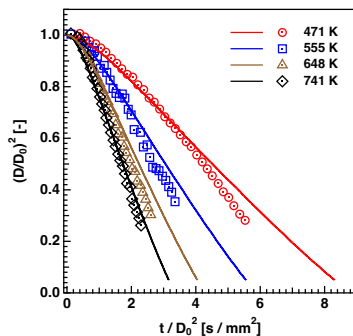


Fig. 1: Comparison of $(D/D_0)^2$ at different temperatures for the evaporation of *n*-heptane. Markers and solid lines indicate the experimental data [2] and numerical results, respectively.

interfacial temperature rapidly rises to about 2350 K at 0.5 ms and approaches a quasi-steady value of about 2500 K at around 2.5 ms. Under the interfacial thermal-equilibrium assumption, evaporation and combustion are diffusion-limited. Vaporized Al is transported outward by diffusion, and its oxidation with O_2 releases heat and raises the flame temperature until a quasi-steady state is established. The predicted quasi-steady flame temperature reaches about 3650 K, in good agreement with recent measurements [3], whereas the interfacial temperature is about 150 K lower, likely because heterogeneous reactions and radiative feedback from Al_2O_3 smoke are neglected.

Figure 3 shows the temporal distribution of the major product $Al_2O_3(l)$. The peak mole fraction of $Al_2O_3(l)$ remains nearly constant at about 0.15 during the first 2.5 ms, while its peak position shifts outward from about 2 to 2.8 particle radii, consistent with the temperature

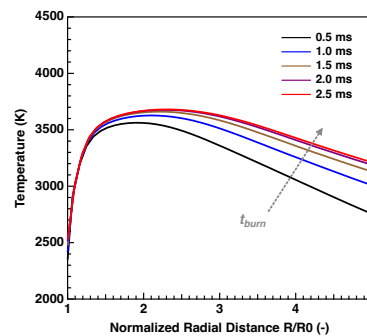


Fig. 2: Evolution of temperature distribution along radial distance.

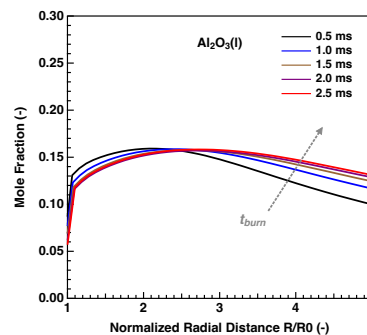


Fig. 3: Evolution of $Al_2O_3(l)$ distribution along radial distance.

peak. Similar outward shifts in both the temperature and $Al_2O_3(l)$ reflect the dominant heat release associated with $Al_2O_3(g)$ condensation, which is modeled through $Al_2O_3(g) \rightarrow Al_2O_3(l)$ reaction.

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Theoretical study of static and dynamic spin structure factors in 3D antiferromagnets

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Precise evaluation of magnetic Hamiltonians is the first step in the study of complex magnetic materials. For 3d materials, DFT+U methods give a very good description, and an energy mapping approach with statistical evaluation of energies of many spin configurations yields excellent results. The mineral nabokoite ($\text{KCu}_7\text{TeO}_4(\text{SO}_4)_5\text{Cl}$) which realizes a square kagome network of Cu^{2+} spins has an intricate hierarchy of exchange interactions that realizes complex spin dynamics on pyramids [1]; theoretical results are in excellent agreement with experiment. By analyzing the spin structure factors for 2D and 3D systems and for different sublattices, we can identify distinct degeneracies and tendencies to form a spin liquid. We also studied $(\text{CsCl})\text{Cu}_5\text{As}_2\text{O}_{10}$ [2] and $\text{Mn}_3\text{Si}_2\text{Te}_6$ [3] using DFT energy mapping and classical Monte Carlo simulations. For $\text{Mn}_3\text{Si}_2\text{Te}_6$, our calculations allow us to precisely capture and explain a dome in the pressure dependence of the ferrimagnetic ordering temperature.

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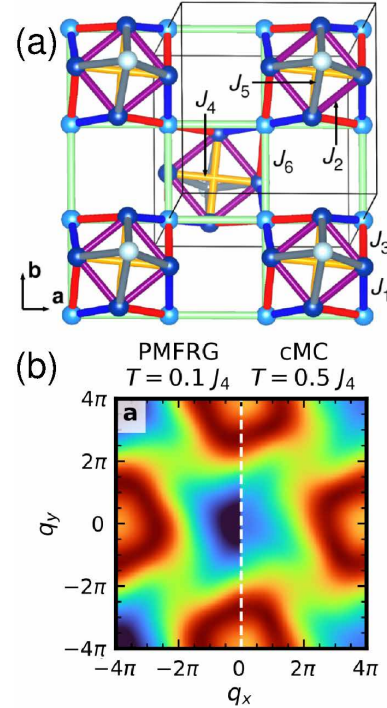


Figure 1: (a) Exchange paths of nabokoite. (b) Quantum and classical spin structure factor.

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Development of tensor network algorithms

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We studied information-theoretic aspects of stochastic time-evolution models using tensor network representations. As a representative nonequilibrium system, we considered the one-dimensional Fredrickson–Andersen (FA) model[1], a kinetically constrained model in which a local spin can flip only when a neighboring site is excited. Although the equilibrium distribution of this model is simple, its dynamical behavior is highly nontrivial. In particular, in the s -ensemble of trajectories, where histories are biased by the dynamical activity, kinetically constrained models exhibit a first-order dynamical phase transition between active and inactive dynamical phases[2].

Our main target was the finite-time transition observed on the $s > 0$ side of the one-dimensional FA model. We analyzed this process with a tensor network simulation of the biased time evolution[3]. Starting from a finite-density state, the system first remains in an active state for a long time and then rapidly approaches an inactive state. The time-dependent density distribution shows a clear bimodal structure for weak bias, such as $s = 0.05$, while it remains essentially single-peaked for stronger bias, such as $s = 0.5$. This contrast indicates that the finite-time transition at weak positive bias can be interpreted as an escape process from a metastable active state in trajectory space.

We then evaluated the second Rényi entropy density of the probability distribution,

$$h_2 = -\frac{1}{N} \log \sum_x P(x)^2,$$

together with the contribution from the zero-density state. The Rényi entropy starts to decrease well before the average density begins to drop at $s = 0.05$. Moreover, its de-

cay is almost dominated by the contribution of the zero-density state. This result shows that the Rényi entropy is sensitive to a structural change in the full probability distribution, even when conventional observables such as the average density still appear to remain in the metastable regime.

These results demonstrate that tensor network methods provide a useful framework for directly evaluating information measures of probability distributions generated by stochastic time-evolution models. The present analysis clarifies the role of the inactive state in the metastable escape process of the s -ensemble and is consistent with the scenario of a first-order dynamical phase transition in kinetically constrained models. As a future direction, we plan to extend the Rényi-entropic analysis to dynamical quantities and to investigate its relation to entropy production and other measures of nonequilibrium irreversibility.

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Partially Entangled Typical Thermal State for Variational Quantum Monte Carlo Calculation

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Random state methods, also known as typical thermal state methods [1-3], have been successfully applied to finite-temperature calculations of quantum many-body systems in the full Hilbert space. The key idea is that the trace of an operator can be approximated by the statistical average of its expectation values over random states,

$$\text{tr}[X] \approx \mathbb{E}[\langle \Phi | X | \Phi \rangle]. \quad (1)$$

The random state method has been extended to *variational wavefunctions* by replacing some of the variational parameters with random variables [4-6]. However, since the number of random parameters is significantly smaller than in the full Hilbert space, the statistical convergence deteriorates, requiring averages over a large number of random states [7, 8].

To address this issue, we propose the *Partially Entangled Typical Thermal State* (PETTS) as a class of random states suitable for finite-temperature Variational Quantum Monte Carlo (VQMC) calculations. PETTS, $|\Phi_{\text{PETTS}}\rangle$, is defined as a tensor product of random states in non-overlapping plaquette subspaces that cover the entire system. It satisfies the trace

formula. (1).

Compared to both fully entangled states in the full Hilbert space and simple product states, PETTS has an intermediate number of random parameters and an intermediate degree of entanglement. As a result, it improves statistical convergence while introducing only a modest increase in computational cost compared to product-state calculations. Examples of plaquette configurations for a 4×4 square lattice are shown in Fig. 1.

For finite-temperature calculations, we consider an extended variational wavefunction defined as the product of a PETTS and a physical ansatz.

$$\Phi(x; \sigma) = \Phi_{\text{PETTS}}(\xi; \sigma) \Phi_{\text{ansatz}}(w; \sigma)$$

where x stands for the combination of ξ and w . The state evolves in imaginary time and thermal expectation values are computed in the same manner as in the full Hilbert space formulation [6]. The most time-consuming part of the calculation, inverting large quantum metric matrices, is efficiently computed using NetKet[9] and JAX[10] on the GPU nodes of System C.

Fig. 2 shows the energy, $E(\beta)$ for each random state in the AFM Heisenberg model on a 4×4 square lattice with $J=1$. A Restricted Boltzmann Machine with $6N_{spin}$ hidden units is used as the physical ansatz. The results demonstrate that stochastic fluctuations are significantly reduced when using PETTS (2×4), compared to the product-state approach.

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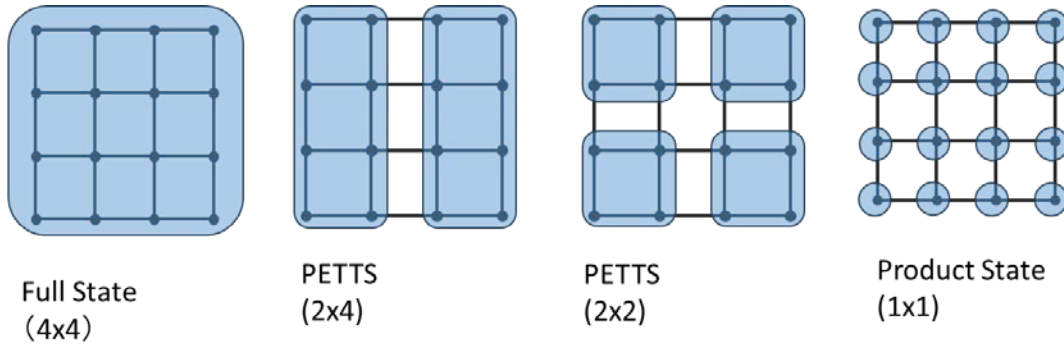


Fig. 1: Examples of plaquette configurations for 4×4 square lattice

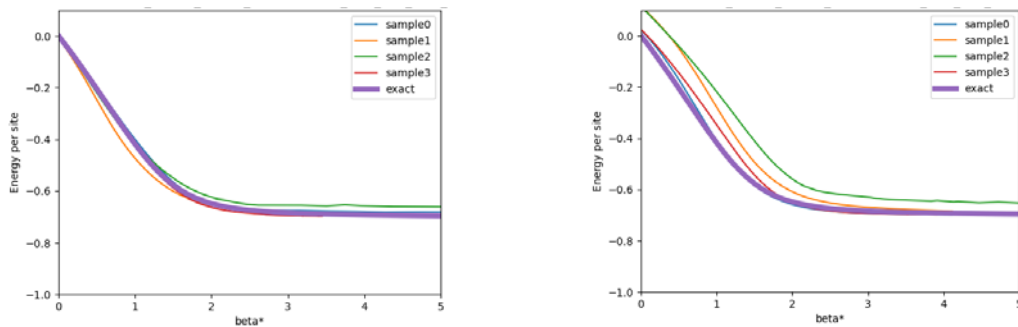


Fig. 2 : Energy, $E(\beta)$ of AFM Heisenberg model on 4×4 square lattice
 (a) PETTS(2×4) (b) Product State

Physical properties of crosslinked polymer networks through network topology analysis

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To investigate the physical/mechanical properties of the crosslinked polymer networks, we studied mainly two types of coarse-grained MD models. (1) Bead-spring type Kremer-Grest (KG) model with bond breakage [1] and (2) Martini force field.

Regarding KG model with bond breakage [1], we studied abnormal butterfly patterns (ABPs) in small angle two-dimensional scattering patterns (2DSPs) of stretched inhomogeneous networks and finalized as a published paper [2]. The product run was performed on FUGAKU on the basis of the preparation study using the ISSP supercomputer. Here, uniaxial stretching was performed under the constant volume condition. Figure 1 (left) shows the ABPs in 2DSPs for stretching ratios $\lambda = 4.0, 4.2, 4.4$, and 4.6 for a diamond lattice network with bimodal strand lengths ($N_s - N_b, N_s + N_b = (10, 40)$). In the large λ regions, a small number of bond breaks occur, gradually increasing the non-uniformity. Reflecting this, the 2DSPs change. Furthermore, in Figure 1 (right), the ABP peak position was evaluated as a function of q_x and it was revealed that it shifts according to the stretching.

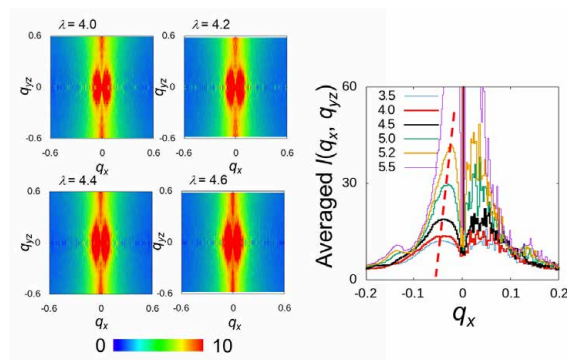


Fig. 1: (Left) ABPs in 2DSPs for stretching ratios of 4.0, 4.2, 4.4, and 4.6, and (right) evaluation of ABP peak shift.

Regarding the Martini force field, we simulated Tetra-PEG gels at eight ($2 \times 2 \times 2$) times the system size of all-atom (AA) models [3]. Despite evaluating stress values across various temperatures and shear strains over 2000 ns, significant noise has hindered systematic results, requiring improved methods to address long-wavelength fluctuations.

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Research of superconductivity induced by multipole fluctuations in the bi-layer orbital degenerate Hubbard model

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In 2023, $\text{La}_3\text{Ni}_2\text{O}_7$ superconductor has been discovered [1], and it was the first bulk superconductor other than cuprates to exhibit a transition temperature T_c higher than the boiling temperature 77K of liquid nitrogen. This material possesses a bilayer Ruddlesden-Popper-type perovskite structure, and the formal valence of nickel ion is $\text{Ni}^{2.5+}$ ($3d^{7/5}$). This is described as a mixed-valence state of Ni^{2+} ($3d^8$) and Ni^{3+} ($3d^7$), corresponding to a configuration in which both the $d_{3z^2-r^2}$ and $d_{x^2-y^2}$ orbitals are half-filled, and a configuration in which only the $d_{3z^2-r^2}$ orbital is singly occupied, respectively.

At ambient pressure, $\text{La}_3\text{Ni}_2\text{O}_7$ does not become superconducting, but when a pressure of 14.0-43.5 GPa is applied, it becomes a superconductor with a maximum T_c of 80 K. According to synchrotron X-ray diffraction (XRD) measurements, $\text{La}_3\text{Ni}_2\text{O}_7$ belongs to the orthorhombic $Amam$ space group under low pressures of 1.6-10.0 GPa, while a structural transition is observed around 10.0 GPa, and at pressures above 15 GPa, it is known to adopt the orthorhombic $Fmmm$ space group. This transition corresponds to a change in the Ni-O-Ni bond angle along the c -axis from 168 to 180 degrees. Accompanying this structural change, the σ -bonding between the Ni $d_{3z^2-r^2}$ orbital and the apical oxygen $2p$ orbital is strengthened. Unlike in cuprate high-temperature superconductors, the $d_{3z^2-r^2}$ orbital is believed to play a crucial role, which is considered one of the characteristic features of

nickelate superconductors.

A large number of theoretical studies have been conducted to clarify the symmetry of the gap function in $\text{La}_3\text{Ni}_2\text{O}_7$ [2–10]. Previous works have shown that the most stable solution is an $s^\pm$ -wave state, originating from interlayer pairing of the $d_{3z^2-r^2}$ orbitals. On the other hand, $d_{x^2-y^2}$ -wave and d_{xy} -wave states are energetically competitive with the $s^\pm$ -wave state, suggesting that the symmetry may change with slight variations in pressure or crystal-field splitting. Experimentally, it remains difficult to precisely determine the gap structure under high pressure, and no definitive conclusion has been obtained. However, point-contact spectroscopy (PCS) measurements have observed a V-shaped spectrum, indicating the possible presence of nodes and suggesting the d-wave gap symmetry [11].

In this research, we analyze the following bi-layer two-orbital Hubbard model for the e_g electron system.

$$\begin{aligned}
 H = & \sum_{\mathbf{k}, \sigma} \sum_{\ell \ell', \mu \mu'} \varepsilon_{\mathbf{k} \ell \ell' \mu \mu'} c_{\mathbf{k} \sigma \ell \mu}^\dagger c_{\mathbf{k} \sigma \ell' \mu'} \\
 & + U \sum_{i, \ell, \mu} n_{i \uparrow \ell \mu} n_{i \downarrow \ell \mu} + U' \sum_{i, \ell} n_{i \ell a} n_{i \ell b} \\
 & + J \sum_{i, \ell, \sigma \sigma'} c_{i \sigma \ell a}^\dagger c_{i \sigma' \ell b}^\dagger c_{i \sigma' \ell a} c_{i \sigma \ell b} \\
 & + J' \sum_{i, \ell} (c_{i \uparrow \ell a}^\dagger c_{i \downarrow \ell a}^\dagger c_{i \downarrow \ell b} c_{i \uparrow \ell b} + \text{h.c.}) \\
 & + U_\perp \sum_i n_{i A b} n_{i B b},
 \end{aligned}$$

where $c_{\mathbf{k} \sigma \ell \mu}$ indicates the annihilation operator of an electron wave vector $\mathbf{k}$ of the layer ℓ

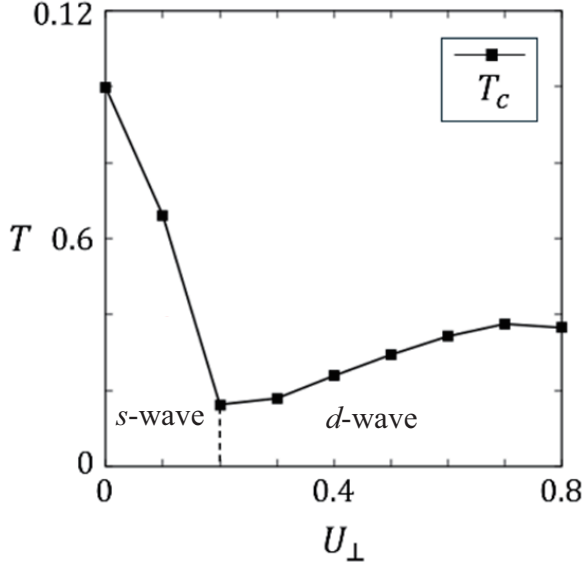


Figure 1: Superconducting phase diagram. With the increase of $U_{\perp}$, the symmetry of the gap function is changed from s - to d -wave.

($=A$ and B) and the orbital μ ($=a$ and b), a and b denote $d_{x^2-y^2}$ and $d_{3z^2-r^2}$ orbitals, respectively, $\varepsilon_{\mathbf{k}\ell\ell'\mu\mu'}$ denotes one-electron energy among layers and orbitals, i indicates the Ni site, $n_{i\sigma\ell\mu} = c_{i\sigma\ell\mu}^{\dagger} c_{i\sigma\ell\mu}$, $n_{i\ell\mu} = \sum_{\sigma} n_{i\sigma\ell\mu}$, U is an intra-orbital Coulomb interaction, U' is an inter-orbital Coulomb interaction, J is an exchange interaction, J' is a pair-hopping interaction, and $U_{\perp}$ denotes an interlayer Coulomb interaction between b orbitals.

In this research, we clarify the effect of $U_{\perp}$ on the superconducting states of $\text{La}_3\text{Ni}_2\text{O}_7$. For the purpose, we solve the gap equation with the effective interaction obtained by a random phase approximation in terms of the Coulomb interactions. As for the details of $\varepsilon_{\mathbf{k}\ell\ell'\mu\mu'}$ and hopping parameters, readers can consult with Ref. [12]. The values of the on-site Coulomb interactions are set as $U = 1.2$, $U' = 0.8$, $J = 0.2$, and $J' = 0.2$ in the unit of eV. The electron number per Ni ion is set as 1.5 throughout the numerical calculations.

A typical results is shown in Fig. 1, in which T_c is depicted as a function of $U_{\perp}$. For $U_{\perp} = 0$, the gap function is dominated by interlayer

pairing of the $d_{3z^2-r^2}$ orbitals, and an isotropic s -wave symmetry is obtained in the orbital representation. This result is consistent with previous studies. For $U_{\perp} \geq 0.2$, the gap function is likewise dominated by interlayer $d_{3z^2-r^2}$ -orbital pairing. Note, however, that the symmetry is found to change to a d -wave state. These results demonstrate that the increase of the interlayer Coulomb interaction $U_{\perp}$ drives a transition in the gap symmetry from an s -wave to a d -wave state.

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Temperature dependence of specific heat in an extended Kitaev model on a honeycomb lattice

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In 2025, we studied the following two projects.

(1) Temperature dependence of specific heat in an extended Kitaev model on a honeycomb lattice

The $S=1/2$ Kitaev- Γ model on a honeycomb lattice is considered as an effective model of RuCl_3 . Numerous efforts have also been devoted to realize materials described by the spin- S Kitaev model and the related model. In this project, we investigated the temperature dependence of the specific heat in $S=1$ Kitaev- Γ model on a honeycomb lattice. In this model, anisotropy exists in the nearest neighbor interaction on each bond as shown in figure 1. In previous project, we clarified the ground state phase diagram and found that the C_3 symmetric phase is lacked in the $N=18$ cluster. Since the C_3 symmetric phase only appears in the $S=1/2$ case under a regular-hexagonal periodic-boundary condition [2], we tried the computation for $N=24$ cluster for the $S=1$ case. However, because the computational cost for $N=24$ cluster is huge, we have not obtained yet enough results to conclude the existence of the C_3 symmetric phase in the $S=1$ case. However, we continue this project to clarify it.

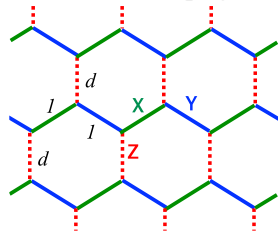


Fig. 1: Anisotropically interacting Kitaev- Γ model. The coupling strength on the X/Y bond is unity, and d is the ratio of the coupling strength on the Z bond against that on the X/Y bond.

Next, we investigated the temperature dependence of the specific heat for the same model in the $S=1$ case by using a thermal pure quantum state [3]. In the $S=1$ case, the two-peak structure is only confirmed near isotopically interacting case ($d \sim 1$) and the two-peak structure disappears as anisotropy of the interaction exists. We find that the single

peak in the spin chain limit corresponds to the high-temperature peak. The obtained results are quite similar to those in the $S=1/2$ case [3].

(2) Temperature classification by machine learning assisted method

In recent condensed matter physics, Machine learning (ML) techniques have been applied to condensed matter physics: ML is applicable to classify phases from a given magnetization distribution [4]. On the other hand, it is known that estimation of temperature from a given magnetization distribution is difficult. This is because similar magnetization distribution appears at different temperatures due to thermal fluctuation. In this project, we focused on the classification of temperatures from given magnetization distribution. First, we prepared data sets of magnetization distribution for several temperatures by classical Monte Carlo calculations for two-dimensional (2d) three-state Potts model on a square lattice. Next, we trained a convolutional neural network by the prepared magnetization distribution, where we adopted a supervised ML method for training. We found that the accuracy of temperature classification is improved when the system size increases and the temperatures are located near the phase transition temperature. In addition, the accuracy of temperature classification shows data collapse with critical exponent for the 2d three-state Potts model, when we perform finite-size scaling analysis.

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Kinetics of phase transition and polyamorphism

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FY2025 was the year in which the author retired. As part of this retirement, he had to shut down his lab during the latter half of FY2025. The author could not substantially access the supercomputer. Therefore, the outcome obtained during the first half, which was reported at the international conference DGK2026, held in Lübeck, Germany, in February 2026, was summarized in this report.

The author has reconsidered polyamorphism, especially a liquid–liquid transition, since 2023. Polyamorphism, by definition, restricts a separation or transition between two states that must consist of a single chemical component. He started the investigation by taking a phosphorus system as an example because it has been established as one that undergoes a transition between thermodynamically stable liquid phases [1]. As reported last year, quantum chemical calculations using GAUSSIAN 19 [2] indicated that approximately 4 eV of activation energy is required to break a single bond in a P_4 molecule to form a radically polymerizable state. That is, the reaction between n P_4 molecules and a $(P_4)_n$ molecule is not physical but indeed chemical. Therefore, the liquid–liquid transition (LLT) in phosphorus could be a monotectic phase transition between two phases composed of different chemical species.

The author examined a similar possibility for SnI_4 , for which he has claimed the presence of the water-type LLT [3] for more than 10 years based on his group’s experimental and theoretical studies, including molecular dynamics simulations. As noted, SnI_4 molecules undergo pressure-induced local sym-

metry breaking prior to the LLT [4]. The author speculated that this symmetry-lowering, which naturally introduces two length scales [4] assumed by the Jagla model [5] used to explain water’s LLT [6], is due to a change in the molecular electronic configuration. GAUSSIAN 19 was again used to find the stable configuration and energy of two SnI_4 molecules approaching each other in a given orientation as a function of the distance between their central tin atoms. (The author performed similar computations already in 2023 without fixing the distance between two molecules. The relaxation finished to push molecules away from a starting distance.) When two molecules approach in an edge-to-edge orientation, the computation allowed the author to calculate the energy until the Sn-Sn distance reached ~ 1 Å, at which point the molecular symmetry lowered from T_d to C_{2v} . The energy increases up to ~ 6 eV at the closest approach. The calculation ended when the molecular distance became 5 Å in a face-to-face orientation. The final energy was slightly less than 1 eV, resulting in squashed C_{3v} molecular deformation. A similar energy–distance relation resulted when two molecules approached in a face-to-vertex (F2V) orientation. The computation was again not converged in this case when the distance decreased below 5 Å. The F2V orientation caused a pair of molecules to deform into squashed, elongated tetrahedra. Experimental measurements confirmed the deformation observed in the computations.

Physical molecular interactions were assessed as follows. First, it was decomposed into three contributions: the dispersion, the

octupole–octupole interaction, and the induced one. The first one was implemented using the four-center Lennard-Jones potential [7], whereas the formula from Ref. [8] was used for the second interaction, leaving the magnitude of the maximum octupole moment as a free parameter. The third interaction was ignored. To the author’s surprise, this assessment based on classical mechanics quantitatively reproduced the quantum-chemical energy–distance relationships obtained under the specified mutual molecular orientations within the distances over which the computations converged. It should be noted that the classical assessment in the F2V orientation showed a peculiar energy–distance behavior at distances beyond the range of quantum assessment; an energy barrier amounting to 30 eV appeared when the intermolecular iodine–iodine separation takes the minimum distance of 2.51 Å. We may conclude the formation of a metallic I₂ bond when two intermolecular iodine atoms approach close within a distance of ~ 3 Å. Therefore, the LLT in SnI₄ may also be a transition associated with a change in chemical components.

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Application of sine-square deformation to calculate thermodynamic properties in frustrated quantum magnets

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We studied finite temperature properties of a quantum spin-1/2 antiferromagnets on two-dimensional lattices. To access bulk behavior with limited system sizes, we employ the sine-square deformation (SSD) technique, where a smooth real-space envelope function continuously suppresses the local energy scale toward the system boundaries. The resulting SSD Hamiltonian yields quantum eigenstates whose central region reproduces bulk-like properties, enabling accurate evaluation of thermodynamic quantities close to the thermodynamic limit even for relatively small finite clusters [1]. Using these effective bulk states, we calculate the temperature dependence of the energy density, specific heat, and magnetic susceptibility [2]. The 1D and square lattice results show agreement with the exact solutions typically within the accuracy of 10^{-3} of the data plotted in Fig. 1. Both the triangular- and kagome-lattice antiferromagnets exhibit characteristic low-temperature anomalies in the

specific heat, including shoulder-like features and pronounced double-peak structures. In contrast, the kagome lattice shows a particularly strong enhancement of magnetic susceptibility extending down to the lowest accessible temperature regime. By comparing these frustrated systems with the square-lattice and one-dimensional antiferromagnets, we clarify the distinct nature of their low-energy excitations. Although both the triangular and kagome lattices retain substantial residual entropy at low temperatures, the excitations below approximately $0.5J$ in the kagome lattice are dominated by magnetic excited states, whereas such magnetic contributions remain much less significant in the triangular-lattice.

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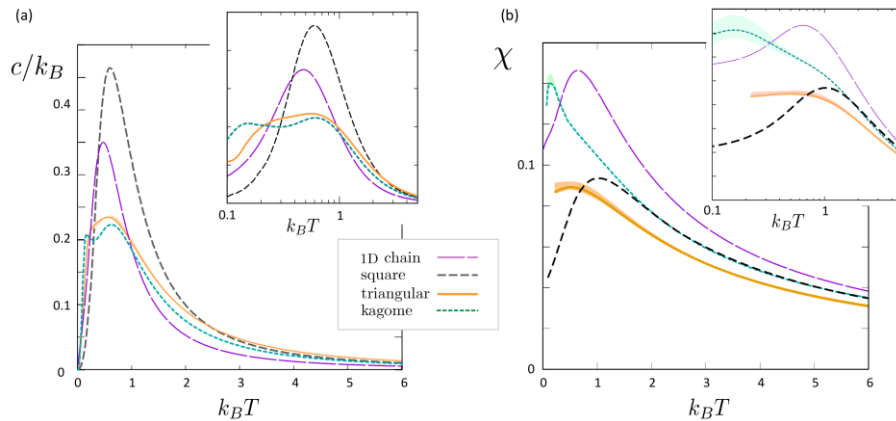


Fig.1: Specific heat and susceptibility of the S=1/2 Heisenberg model on four different lattices.

Stabilization of borophene by step edges on Ni(111)

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We have investigated the formation of borophene on the Ni(111) surface. Experimental scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED) results indicate that B₁₃ borophene is formed, which is supported by corresponding theoretical simulations. However, density functional theory (DFT) calculations using VASP, combined with structural searches based on particle swarm optimization (CALYPSO) [1], suggest that B₁₃, B₁₄, and B₁₅ borophene structures are energetically competitive, as shown in Fig. 1(a).

To reconcile these experimental and theoretical results, we further examined the formation energies of borophene at step edges. Figure 2 shows the structural models for B_n (n

= 12–17) with Ni [-110] steps. The angles between the step edges and the borophene frameworks are also indicated. The adsorption energy per boron atom is lowest for the B₁₃ structure, as shown in Fig. 1(b). The formation energies, including the effect of step edges, further support the stability of the B₁₃ structure.

These results demonstrate that borophene is stabilized at Ni step edges, which broadens the structural diversity of two-dimensional borophene sheets and provides new insights into the controlled synthesis of complex borophene architectures at step edges [2].

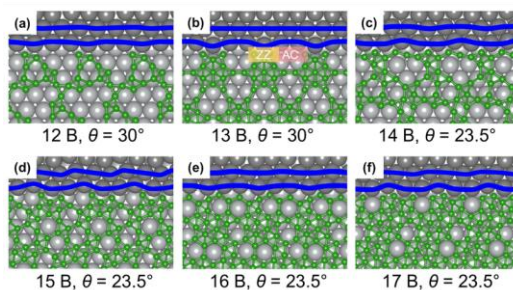


Fig. 1. Structural models for B_n (n = 12–17) with Ni [-110] steps. The angles between the step edges and the borophene frameworks are also indicated.

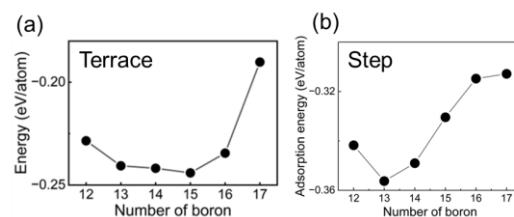


Fig. 2. Adsorption energy for B_n (n = 12–17) borophene models (a) on terrace and (b) terrace a with Ni [-110] steps. The angles between the step edges and the borophene frameworks are also indicated.

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Enhancement of correlation functions due to deficit in quantum spin systems

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In a square-lattice antiferromagnetic Heisenberg model consisting of coupled bond-alternating chains of spin size $S = 1/2$, the ground state becomes an antiferromagnetic long-range ordered state and a dimerized state depending on the strengths of the bond alternation and interchain interaction. Dilution effects on the systems have been investigated using a quantum Monte Carlo method [1,2]. In the antiferromagnetic long-range ordered phase of the system without bond alternation, the finite staggered magnetization decreases monotonically with increasing the concentration of site dilution, and reaches zero at the percolation threshold. On the other hand, in the dimer phase, the finite staggered magnetization is induced by dilution. Interestingly, near the parameter where a quantum phase transition is driven in the pure system, it has been reported that the staggered magnetization does not decrease due to site dilution but increases once, even though the phase is antiferromagnetic long-ordered phase [1].

In this project, we calculated spin correlation functions of the ground state in the bond-diluted antiferromagnetic Heisenberg model consisting of bond-alternated chains on a square lattice using the quantum Monte Carlo method with the continuous-imaginary-time loop algorithm. In the loop algorithm, spin correlation functions between two spins can be calculated efficiently by an improved estimator. In order to investigate relations between the staggered magnetization and the spin correlation function, we examined the change in the distribution of

the correlation functions with dilution in a randomly diluted bond system. At the concentration of dilution where the staggered magnetization is increased, the distribution of the nearest-neighbor correlation functions changed significantly compared to those of other correlation functions. However, no significant change was observed in the distribution due to the bond alternation and interchain interaction. Further investigation is needed.

In the process of this research, we found that all nearest-neighbor spin correlation functions are enhanced in a 1/8-depleted lattice system. The system is obtained by periodic site dilution in a square-lattice antiferromagnetic Heisenberg system and is composed of bipartite sublattices. Since the numbers of spins on the A and B sublattices are different due to the 1/8 depletion, the 1/8-depleted lattice system exhibits ferromagnetic properties. We investigated the phase-transition temperatures in quasi-two-dimensional systems with 1/8-depleted lattices as the two-dimensional plane using the quantum Monte Carlo method. Our results establish a universal relation between the phase-transition temperatures and the inter-plane interactions [3].

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Analyses on the dynamics of metal ion solutes in ionic liquid-based electrolytes at the interfaces

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Ionic liquids (ILs) are promising electrolytes for electrochemical devices such as secondary battery, capacitor, etc., due to their high chemical stability with negligible vaporization. Structuring and dynamics of the interfacial IL faced to charged graphite electrodes have been analyzed by molecular dynamics (MD) calculations [1], but the transport of Li^+ ion inside EDL formed at negatively charged electrode is not apparent because Li^+ coordinated with anions has negative charge in total. Recent our interface-selective spectroscopic study (EC-ATR-FUV) revealed such ion dynamics at the electrified interface [2], but molecular view is still insufficient. In the present study, we have analyzed the transport of Li^+ ion inside EDL of a BMIM-TFSI ionic liquid electrolyte at the negatively charged graphite electrode by MD calculations, which is closely related to charging process of Li-ion battery composed of these components.

All MD simulations were conducted by classical MD package of LAMMPS. A simulation cell contains 650 ion pairs of BMIM-TFSI with randomly distributed 150 pairs of Li-TFSI ($9 \times 8 \times 11 \text{ nm}^3$) sandwiched with 5-layer graphite electrodes from top and bottom separated with vacuum layer. The same amounts of positive and negative charges were assigned to the top and bottom electrodes, respectively at the graphene layer faced to the electrolyte reproducing the electrified interfaces. In Fig. 1, interface structure obtained by following two different applied potential sequences; (i) firstly stabilized the interface structure by annealing the cell at the surface charge equivalent to $\pm 1.8 \text{ V}$ and then the surface charge equivalent to $\pm 3.5 \text{ V}$ was applied (lower case in Fig. 1) and (ii) the surface charge equivalent to $\pm 3.5 \text{ V}$ was directly applied (upper case in Fig. 1). MD trajectories

for 10 ns at 350 K were analyzed.

Apparent difference was found for the interface structure at the electrode potential of -3.5 V depending on the applied potential sequences (Fig. 1). By the sequence (ii), no Li^+ was present close to the electrode. By analyzing the MD trajectories, it was due to the dense BMIM cation layers already formed by equilibrium at -1.8 V , which prevent the exchange of Li^+ at least during 10 ns. In the sequence (i), the interface is rather randomized and provided the chance for some Li^+ to be attached to the electrode by deforming the coordination with TFSI anions in 10 ns.

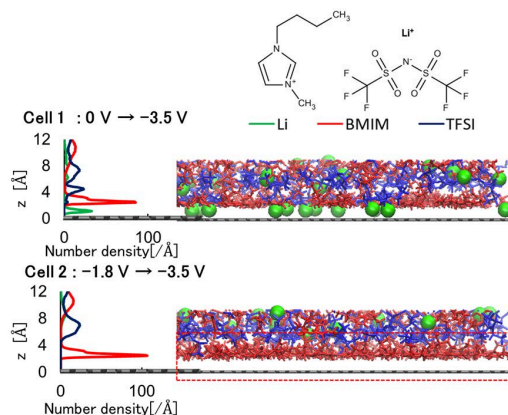


Fig. 1 Applied-potential-sequence dependent interfacial structure of a Li^+ containing BMIM-TFSI electrolyte at -3.5 V vs. PZC by MD calculation.

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Self-organization and dynamics in dendrimer polyelectrolytes

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Dendrimers are macromolecules characterized by molecular chains that extend radially from the center of the molecule through repeated branching [1]. Due to their unique tree-like architecture, they possess precisely controlled shapes and functions at the molecular level. Molecular dynamics simulations of charged dendrimer systems have been conducted to investigate their structural formation. Karatasos [2] performed such simulations on charged dendrimer solutions with varying surface charge densities. The study reported that systematic variations in the Bjerrum length induce a mechanism related to the spatial correlation of counterions, driving the system from an amorphous, liquid-like arrangement to an ordered state with cubic phase symmetry.

However, this previous research was performed on a very small system consisting of only 30 molecules. Since order formation in soft matter is significantly affected by finite-size effects, it is of great interest to perform large-scale computer simulations using parallel supercomputers to better study this phenomenon in dendrimers.

In this study, the structure formation of charged dendrimer systems was investigated through parallel molecular dynamics

simulations using LAMMPS. The simulated system contained 1,600 molecules. Evaluation of the generalized local order parameter [3] and the structure factor revealed that the system did not undergo crystallization even at high densities, instead remaining in a random configuration (Fig. 1). The identification of a crystalline phase remains an important subject for future investigation.

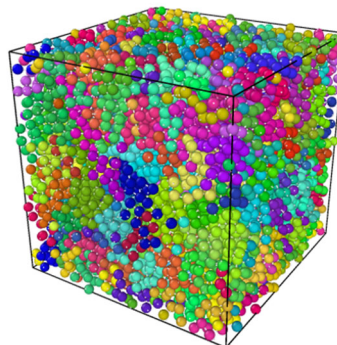


Fig. 1: Snapshot of the dendrimers with $\rho\sigma^3 = 1.25$.

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Shape dependence of dynamic friction in viscoelastic materials

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In this project, we investigate dynamic sliding friction in viscoelastic solids by finite element simulations. Frictional behavior of viscoelastic materials is computed over a wide range of viscosity coefficients and for sliding velocities from low speeds up to the elastic wave speed scale.

The simulations are executed on System C kugui using MPI-based domain decomposition of the finite element mesh. A typical run uses 16 compute nodes (2,000 cores) for 24 hours, solving a problem with 10 million finite-element nodes and 100 million time steps using our in-house code compiled with the Intel Fortran compiler.

As shown in Fig. 1, we show that the friction coefficient μ varies depending on the material viscosity $\tilde{\eta}$, and that the critical velocity where μ reaches a peak changes systematically. In particular, for low viscosity, the singular deformations occur at sliding velocities near the sound speed, resulting in rapid increases around the Rayleigh wave speed $\tilde{c}_R$ and rapid decreases around the longitudinal wave speed $\tilde{c}_L$ in the friction coefficient that cannot be

explained solely by viscous effects. Based on the findings obtained in this study, we are further investigating the effect of geometric factors, such as contact shape, on frictional behavior.

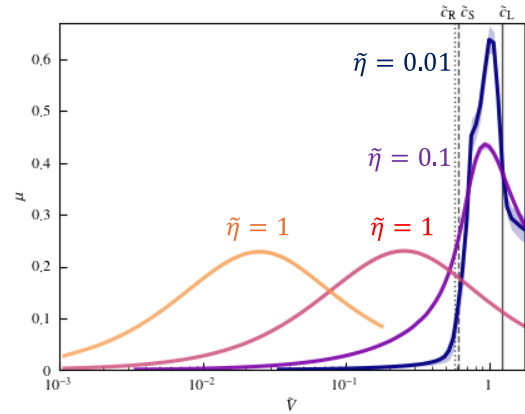


Fig. 1: Dependence of friction coefficient μ on sliding velocity $\tilde{V}$ for different viscosity coefficients $\tilde{\eta}$. The vertical lines represent the Rayleigh wave speed $\tilde{c}_R$, shear wave speed $\tilde{c}_S$, and longitudinal wave speed $\tilde{c}_L$.

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Numerical Study of Dynamics in Spin Systems

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In this project, we continued numerical studies related to Kitaev spin systems from several complementary directions. As a recent outcome along this line, we studied the spin Seebeck effect in Kitaev spin liquids and clarified characteristic spin-current responses associated with fractional Majorana excitations [1]. This study also highlighted the importance of investigating dynamical and transport properties in a broader class of spin systems beyond the Kitaev limit, and provided useful background and motivation for the present project.

A main subject of the present project is a model interpolating between the AKLT state and the Kitaev spin liquid. Since the original honeycomb-lattice problem is computationally demanding, we started from a two-leg ladder geometry and developed a finite-system DMRG code for this purpose. The implementation was based on the ITensor library [2]. During this project period, the main emphasis was placed on establishing the numerical framework, carrying out benchmark calculations against exact diagonalization for small systems, and performing preliminary calculations for larger ladder systems. We also initiated a basic survey of the evolution between the AKLT and Kitaev limits for both ferro- and antiferromagnetic Kitaev couplings, as a step toward a more systematic analysis in future work.

Another important direction of the present project was international collaborative studies of spin systems using quantum Monte Carlo and related analytical approaches, including coupled-dimer antiferromagnets [3]. In partic-

ular, these studies clarified characteristic dynamical responses and field-induced features in such systems, providing a useful point of comparison for the spin-dynamical aspects of the present project. They also helped refine our perspective on spin dynamics and on the interpretation of numerical results obtained in the present study.

Further related results were presented at the 2025 Hokuriku Branch Meeting of the Physical Society of Japan. These included real-time simulations of current response in a classical Kondo lattice model with a helical spin structure and a study of the stability of vortex-antivortex crystals in a two-dimensional XY model with variable interaction range and magnetic field. Based on these results and ongoing collaborative work, we identified a concrete direction for extending the present project toward dynamical phenomena in both insulating and metallic magnetic systems.

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Theoretical study on cooperative phenomena between magnetism and superconductivity in electron systems with multiple degrees of freedom

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We have theoretically studied the interplay between superconductivity and magnetism in strongly correlated electron systems, by using numerical methods of microscopic models with multiple degrees of freedom including quantum many-body calculations as well as phenomenological analyses (project number: 2025-Ba-0006). During the last fiscal year, we have achieved some progress on the following topics.

(1) Phase-modulated superconductivity coexisting with altermagnetism

We conducted a study on spatially nonuniform superconducting states coexisting with altermagnetism [1], which induces anisotropic spin splitting in the energy bands despite a collinear antiferromagnetic structure. We performed many-body calculations of a Hubbard model on a two-sublattice tetragonal lattice, which incorporates a molecular field of the altermagnetic order and describes the anisotropic spin splitting. To discuss superconductivity mediated by magnetic fluctuations, we analyzed the linearized Eliashberg equation based on the random phase approximation. In this analysis, we employed the Matsubara Green's function method and utilized the `SparseIR.jl` package [2], which is based on the intermediate representation [3] and the sparse sampling [4], to reduce memory usage and computation time. As a result, we demonstrated that Fulde–Ferrell–Larkin–Ovchinnikov (FFLO) superconductivity, a spatially nonuniform state characterized by a finite center-of-mass momentum, is stabilized in the presence of altermagnetism.

Next, we microscopically constructed the phe-

nomenological Ginzburg–Landau (GL) theory for superconductivity in altermagnets. The GL free energy density in tetragonal systems is represented by

$$f = \alpha|\eta|^2 + \beta|\eta|^4 + \kappa|\nabla|^2 + \delta|\nabla^2\eta|^2 + \delta'|\partial_x\partial_y\eta|^2,$$

up to the fourth order of the superconducting order parameter η and spatial derivatives ∂_i . We numerically determined the coefficients α , β , and κ of the GL free energy, and revealed that κ (the second-order gradient term) changes its sign from positive to negative as the molecular field of altermagnetism increases, while β (the fourth-order uniform term) remains positive. Consequently, the FF state, in which only the *phase* of the order parameter is spatially modulated, is induced by altermagnetism. This is in contrast to the well-known result that the *amplitude*-modulated LO state is stabilized under a uniform Zeeman field, where both κ and β almost simultaneously change their sign. Thus, we conclude that the altermagnetism-induced FF state manifests itself as a novel type of exotic superconductivity that had not been previously identified.

(2) Magnetic excitations in heavy-fermion spin-triplet superconductors

We studied magnetic excitation spectrum, which can be observed by inelastic neutron scattering experiments, in the heavy-fermion multiband superconductor UTe_2 [5]. We numerically calculated the dynamical spin susceptibility, within the random phase approximation, of a mixed-dimensional periodic Anderson model [6] that reproduces the antiferromagnetic fluctuations observed near $\mathbf{Q}_{\text{AFM}} = (0, \pi, 0)$ in UTe_2 . In the normal state, we showed

that the hybridization between the conduction and localized f electrons gives rise to a magnetic resonance at $\mathbf{Q}_{\text{AFM}}$, which is enhanced by the quasi-one-dimensional structure of the conduction bands. Furthermore, we demonstrated the resonance in the dynamical spin response due to the superconducting feedback effect when the order parameter belongs to the B_{2u} representation, which changes its sign upon momentum transfer of $\mathbf{Q}_{\text{AFM}}$. The enhancement of the spin response is shaped by the orbital-dependent coherence factor, and the sign reversal of the order parameter determines whether the dynamical spin susceptibility is reinforced or suppressed.

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Hyperuniformity in generalized Aubry-André model

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We have studied a generalized Aubry-André (GAA) model [1] in terms of hyperuniformity (HU) [2], extending our previous study [3] on the genuine Aubry-André (AA) model [4]. The HU is a framework originally proposed to quantify and classify point distributions in a space. It provides a measure for a uniformity of the point distributions, and classify them into several distinct classes, such as nonhyperuniform, and hyperuniform class I, II and III, characterized by a large-scale behavior of the point-density fluctuation. The framework has been generalized to a scalar field, which allows us to characterize the inhomogeneous electron distributions in quasiperiodic systems.

The GAA Hamiltonian reads

$$\hat{H} = t \sum_i \left(\hat{c}_{i+1}^\dagger \hat{c}_i + \text{H.c.} \right) + \sum_i V_i \hat{c}_i^\dagger \hat{c}_i. \quad (1)$$

where $\hat{c}_i^\dagger$ ($\hat{c}_i$) is the creation (annihilation) operator of a spinless fermion (electron) at site i . The parameter t denotes the nearest-neighbor hopping amplitude, and

$$V_i = \lambda \frac{\cos(2\pi i/\tau)}{1 - \alpha \cos(2\pi i/\tau)} \quad (2)$$

with $\tau = \frac{1+\sqrt{5}}{2}$ (golden mean) is the onsite potential, where the overall scale is set by λ while an additional modulation is introduced by $\alpha \in (-1, 1)$.

In Ref. [3], we have shown that inhomogeneous charge distributions in the AA model, which corresponds to $\alpha = 0$ in the GAA model, are hyperuniform: For $\lambda < 2|t|$, the electron states are extended and the charge distribution is class-I hyperuniform, whereas for $\lambda > 2|t|$ the electron states are localized and the charge

distribution is class-II hyperuniform, depending on whether the Fermi level lies inside a gap or not. We examined this notion in the GAA model.

By using the ISSP Supercomputer System B, we explored various sets of parameters (λ, α) . We diagonalized the Hamiltonian Eq. (1) of 46368 sites, which is the 23rd Fibonacci number, calculated the charge distribution and its HU class. We find that the HU class is I (II) when the Fermi level is in the gapless region and the electron state at the Fermi level is extended (localized); In the gapped region the HU class is always I. These are true even when the Fermi level is above the mobility edge, which exists in the GAA model unlike the AA model, where both extended and localized states contribute to the charge distribution.

These results clarify a close relationship between the extended/localized nature of the electron states and the HU class of the charge distribution in quasiperiodic systems.

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Physical properties of Ising machines

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We have continued our studies on the physical properties and computational performance of Ising machines, with a particular focus on quantum annealing (QA). QA is a metaheuristic for solving combinatorial optimization problems by searching for the ground state of an Ising-type problem Hamiltonian, and elucidating its physical mechanisms and limitations is essential for the practical use of current and future quantum hardware. This year, we addressed three complementary aspects: (i) a quantitative analysis of the effectiveness of mid-anneal measurement (MAM) in constrained combinatorial optimization [1], (ii) the application of MAM to multi-objective optimization (MOO) on a physical quantum annealer [2], and (iii) the acceleration of QA in small-energy-gap instances by introducing controlled diagonal catalysts [3].

In the first study [1], we introduced a quantitative metric Q_d to evaluate the effectiveness of MAM. Numerical simulations of the graph bipartitioning problem and the quadratic knapsack problem, formulated using the augmented Lagrangian function, revealed that MAM is most effective when the energy

difference between the desired (feasible/optimal) solutions and the ground state of the problem Hamiltonian is small. Through additional analysis on fully connected Ising models exploiting their permutation symmetry, we further demonstrated that this effectiveness persists as the system size increases, indicating the scalability of MAM toward large-scale quantum annealing.

In the second study [2], we extended this idea to multi-objective optimization, where the conventional linear weighted-sum method inherently fails to reach solutions located in non-convex regions of the Pareto front. We validated the proposed MAM-based scheme through complementary approaches: physical experiments on a D-Wave Advantage2 quantum annealer using quench-based readout, and numerical simulations of closed quantum systems assuming ideal MAM. Both consistently exhibited a clear trade-off in which earlier measurement timing enhances solution diversity, whereas later timing ensures convergence to non-dominated solutions, with a practical compromise timing balancing both metrics.

In the third study [3], we proposed a method

that introduces additional longitudinal magnetic fields as controlled diagonal catalysts to mitigate the small energy gaps that arise from perturbative crossings. By variationally optimizing only the schedule of these linear catalyst terms via optimal-control theory, we demonstrated an approximate quadratic speedup of the exponential scaling exponent of the time-to-solution for the maximum weighted independent set problem on complete bipartite graphs, by actively exploiting diabatic transitions in the small-gap region. We further confirmed that the optimized catalyst schedules are transferable across instances sharing a similar energy-gap structure, suggesting a route to eliminate per-instance optimization overhead.

In all three studies, the time-dependent Schrödinger equation was integrated using QuTiP, and the large-scale numerical simulations were carried out on the System B supercomputer at SCC-ISSP.

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Tensor Renormalization Group Calculation of Universal Values of Partition-Function Ratios

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The tensor renormalization group (TRG) method is a numerical method for approximating the contraction of tensor networks by performing coarse-graining corresponding to the real-space renormalization group [1]. Since the tensor network representation of the partition function can be obtained relatively easily even for complex systems, it is expected to be able to handle systems and physical quantities that are difficult to calculate by conventional methods such as Monte Carlo methods. Recently, a method called bond-weighted tensor renormalization group (BWTRG) was proposed, which significantly improves the calculation accuracy without increasing the computational cost by leaving a diagonal matrix called bond weight on the bond connecting the tensors [2].

In the numerical analysis of phase transitions and critical phenomena, the critical temperature and critical exponent can be calculated with high accuracy by using dimensionless quantities such as the Binder ratio. Since the partition function can be calculated directly by TRG, a dimensionless quantity defined from the ratio of partition functions,

$$X_1 = \frac{Z(L, L)^2}{Z(2L, L)}$$

is useful [3]. This dimensionless quantity proposed by Gu and Wen can extract the information of the tensor corresponding to the fixed point of the renormalization group by canceling out redundant correlations on loops in the numerator and denominator. Therefore, it can detect phase transitions by jumping in value

before and after the transition point in the thermodynamic limit.

In this study, we investigate the behavior of the partition-function ratio near the critical point and find that it follows a scaling law of the same form as the Binder ratio, and that the universal value at criticality is expected from the modular invariant partition function in conformal field theory [4]. We perform numerical calculations using BWTRG in three two-dimensional models belonging to different universality classes: the Ising model, the three-state Potts model, and the four-state Potts model. We verify their behavior near the transition point and clarify the bond-dimension dependence of the calculation accuracy. In particular, in the 4-state Potts model, logarithmic corrections to finite-size effects can be directly observed, which is an example showing the usefulness of tensor renormalization group. We also consider anisotropic systems and show that the correlation length ratio can be estimated from the universal value of the partition function ratio.

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Phase structure and rheology in polymer blends: A molecular dynamics simulation study

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Polymer blends are typically immiscible and exhibit phase-separated structures. Such blends are widely used in polymer products, such as multilayer films. To design sophisticated products, it is necessary to understand the fundamental phenomena associated with phase-separated structures under an external field. Regarding this point, Macosko and coworkers measured the shear viscosity (η) of a laminated system of two immiscible polymers.[1] They reported that η decreased with increasing layer number, attributing this decrease to slip at the interface. To investigate interfacial phenomena at the microscopic scale, this study examined the shear rheological properties of immiscible polymer multilayer systems using coarse-grained molecular dynamics (CGMD) simulations.

This study used the Kremer-Grest (KG) model, a standard CGMD model for polymers.[2] The KG model represents polymer chains by a series of beads connected by finitely extensible nonlinear elastic springs. We introduced a Lennard-Jones (LJ) potential with interaction strength ϵ_{ij} ($i, j \in \{1, 2\}$) for all bead pairs of polymers 1 and 2. To systematically adjust polymer compatibility, we varied the LJ parameter (ϵ_{12}) across polymers. To apply shear flow, solid walls were placed at the top and bottom of the computational domain in the z -direction. Different types of polymers were stacked in the z -direction with 2 or 4 layers. For the equilibrated system, we applied shear flow by

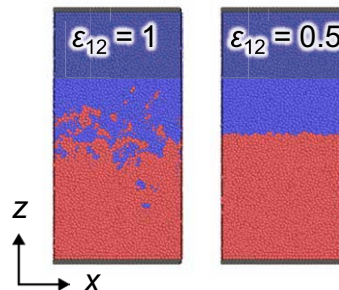


Figure 1: Snapshots of KG simulations for different ϵ_{12} values as indicated.

moving the walls at a constant velocity in the x -direction. Then, the mechanical responses, such as η , were investigated. We conducted all KG simulations using LAMMPS.

We constructed a system consisting of 400 polymer chains, each with $N = 100$, in each layer. By decreasing ϵ_{12} from its standard value of 1, we reproduced a clear phase-separated state in equilibrium, as shown in Fig. 1. From the phase-separated profile, we estimated the Flory-Huggins interaction parameter (i.e., χ parameter). When we applied shear flow to these equilibrium structures, the steady-state viscosity η decreased over a wide range of shear rates as ϵ_{12} decreased (i.e., as the χ parameter increased). This observation qualitatively agrees with the experimental results by Macosko and coworkers.[1]

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Tensor-network approach to phase transition of quantum chiral spin model

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Classical spin models of monoaxial chiral magnets exhibit a continuous phase transition (CPT), known as the Dzyaloshinskii transition, driven by chiral solitons under magnetic fields perpendicular to the helical axis. Below the saturation field, chiral solitons form a periodic array, and the inter-soliton distance, determined by their repulsive interactions, diverges logarithmically. In tilted magnetic fields, two multicritical points appear, leading to discontinuous phase transitions (DPTs) in intermediate angular regions due to attractive soliton interactions.

In quantum monoaxial chiral magnets, several quantum effects have been identified, such as spin parity effects in small systems with periodic boundary conditions and quantum tunneling across surface barriers. Concerning the phase transitions under tilted magnetic fields, quantum fluctuations strongly modify the classical behavior: the discontinuous region disappears for $S = 1/2$, while it remains for $S = 1$ and $S = 3/2$, although it is significantly reduced. Nevertheless, the critical behavior of the Dzyaloshinskii transition in the quantum regime has remained unclear.

In this project, we investigate magnetization processes and phase transitions in quantum monoaxial chiral magnets under tilted magnetic fields using tensor network methods, focusing on the higher-order tensor renormalization group (HOTRG). This year, we have improved the HOTRG implementation, including a more accurate evaluation of excitation

energies and a refined method for extracting excitation gaps. These developments enable a highly precise determination of critical points from gap-closing behavior.

Based on this improved approach, we have successfully determined the critical behavior of the Dzyaloshinskii transition in the quantum $S = 1/2$ case. Although the magnetization curves exhibit a sharp increase just below the transition point, similar to the classical case, the criticality is qualitatively different. Instead of the logarithmic singularity characteristic of the chiral soliton lattice in classical systems, the magnetization approaches saturation in a power-law manner. We further confirm that the quantum $S = 1$ case exhibits the same power-law critical behavior with an identical critical exponent.

Furthermore, we find that this power-law critical behavior is universal across all field angles, indicating that the critical exponent is independent of the tilt angle.

Numerical Simulation of Microwave Response for Fractional Quantum Hall droplet

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The fractional quantum Hall effect (FQHE) has had a profound impact on condensed matter physics. Thanks to significant advances in nanofabrication and measurement technology, this fractional statistics has recently been directly verified through Fabry–Pérot interferometry and nonequilibrium noise measurements [1, 2]. Previous studies have focused on transport properties such as current and nonequilibrium noise in devices where a quantum point contact (QPC) or an interferometer is fabricated in the edge channel. Against this background, probing edge excitations via microwave absorption in an isolated quantum Hall droplet is expected to provide a fundamentally new experimental window distinct from conventional transport measurements.

We numerically evaluated the microwave response of edge states in a system composed of a droplet in the fractional quantum Hall state (Laughlin state) coupled to a microwave waveguide [3]. The system considered in this study was theoretically proposed in a previous work [4] as a setup capable of observing the anyonic statistics of excitations in the edge states. Our numerical results are expected to enable detailed comparisons with future experimental results.

We formulated the effective action of the system by assuming a circular droplet and employing bosonization. The response function to be calculated involves the correlation function of the bosonic field describing the edge states. Since this correlation function cannot be ob-

tained analytically, we performed numerical calculations using the path-integral quantum Monte Carlo method using large-scale parallel computations on ISSP supercomputer. We numerically evaluated the response functions for two cases: a fractional quantum Hall droplet with Landau level filling factor $\nu = 1/3$, $\nu = 1/5$, and an integer quantum Hall droplet with $\nu = 1$, for which analytical theoretical construction is possible. In the numerical simulations, we performed 30,000 Monte Carlo steps for thermalization, followed from 1×10^6 to 1.2×10^6 steps for measuring the correlation functions.

The results of our numerical calculations are presented below. Figure 1 and 2 show the coupling dependence of the response function for the case of Landau level filling factor $\nu = 1/3$, $\nu = 1/5$ and $\nu = 1$. These results show that the peak position depends on the coupling strength, and that this dependence becomes increasingly pronounced as the filling factor decreases, indicating that higher-order contributions become more significant at smaller filling factors. This leads to an enhanced peak shift. This behavior has not been reported in previous studies, including Ref. [4], and thus represents a novel finding.

In the future, we plan to extend our analysis from simple droplet geometries to annular systems with a nontrivial topology. By evaluating the microwave response in such geometries, we aim to clarify how the unique properties of anyons manifest in the optical response of sys-

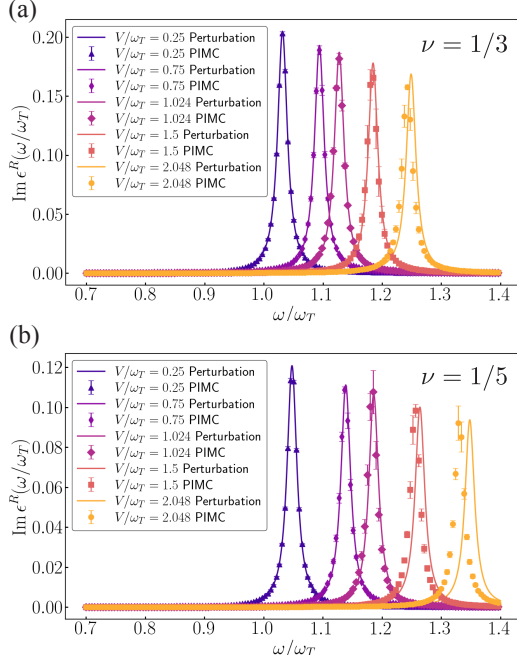


Figure 1: Imaginary part of the dielectric function for FQH droplets with (a) $\nu = 1/3$ and (b) $\nu = 1/5$ at temperature $T/\omega_T = 0.1$. Solid lines show results from second-order perturbation theory, whereas symbols with error bars represent data obtained using PIMC. Coupling strengths are $V/\omega_T = 0.25, 0.75, 1.024, 1.5$, and 2.048 . A finite broadening $\delta = \omega_T/100$ is used.

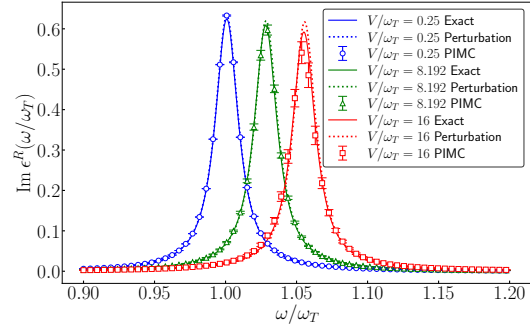


Figure 2: Imaginary part of the dielectric function for the $\nu = 1$ IQH droplet, shown in units of L^2/ω_T . The temperature is set to $T/\omega_T = 0.1$. Solid and dashed lines show the results of scattering theory and second-order perturbation theory, respectively, while symbols with error bars represent numerical data obtained using the PIMC method. Dimensionless coupling strengths are $V/\omega_T = 0.25, 8.192$, and 16 . For visual clarity, delta functions are broadened into Lorentzians with linewidth $\delta = \omega_T/100$.

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Non-reciprocal neighbor interaction and non-equilibrium phase transition in self-propelled hard polygon systems

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Hard disk and sphere systems are among the most fundamental models in statistical mechanics, with a long history of molecular simulation studies spanning equilibrium and non-equilibrium phenomena [1]. In this project, we explore equilibration dynamics and non-equilibrium phase transitions in self-propelled hard particle systems using advanced computational methods: Event-Chain Monte Carlo (ECMC) [2, 3], Newtonian Event-Chain Monte Carlo (NECMC) [4], and Event-Driven Molecular Dynamics (EDMD) [5].

Crystallization and Motility-Induced Phase Separation in the Flow of Active Brownian Particles Around an Obstacle [6]: Fluid-obstacle interactions are central to fluid dynamics, from the Kármán vortex street to Reynolds number-dependent instabilities. While well characterized via Navier-Stokes simulations and classical molecular dynamics, the behavior of active matter under analogous conditions remains largely unexplored. Through large-scale simulations of active Brownian particles (ABPs) flowing past a fixed obstacle, we discover novel emergent patterns including unexpected crystallization. These phenomena are governed by both Reynolds number and self-propulsion velocity, with crystallization arising from two distinct mechanisms: compression-induced ordering upstream and motility-induced phase separation in specific flow regions.

Self-organized spatial inhomogeneity in self-

propelled quasi-elastic hard disk systems [7]: Freely cooling inelastic hard sphere systems serve as a primal model for granular gases. Using large-scale molecular dynamics simulations, we explore the emergence of self-organized spatial structures in quasielastic hard disk systems. Across high-density regimes near the Alder transition, we uncover previously unreported dynamical behaviors and striking spatial patterns. We further assess the influence of different velocity scaling schemes on the observed dynamics. These results offer fresh perspectives on self-organization phenomena in dense quasielastic hard disk systems.

Cooperative phenomena in active matter systems with alternative interaction of neighbors [8]: We examine how nearest neighbor (NN) determination methods affect flocking phase transitions in the Vicsek model. Beyond conventional approaches (Cutoff, Voronoi, k-NN), we introduce 2D SANNex [9], a novel method. While metric-free Voronoi maintains a constant transition point across densities, both k-NN and 2D SANNex exhibit density-dependent shifts despite also being metric-free. This reveals that the metric-free property alone does not govern density dependence; rather, the non-reciprocal characteristics inherent to k-NN and 2D SANNex play a crucial role in modulating transition behavior.

Quantitative analysis of pedestrian counter-flow in crowded condition using floor field

model [10]: Building upon the model by S. Nowak and A. Schadschneider (Phys. Rev. E, **85**, 066128 (2012)), which analyzed lane formation and gridlock in pedestrian counter-flows using the floor field model, we extended the framework from a square lattice (4-directional) to a triangular lattice (6-directional) and compared the phase diagrams of both systems. We further applied these models to pedestrian crossing flows at T-junctions, examining differences in crowd formation using two static floor fields.

Flyer-Target simulation of shock waves in crystal-fluid impact in hard disk systems: Shock waves from supersonic impacts induce phase changes in crystalline materials under extreme compression, but conventional Navier-Stokes simulations cannot resolve particle-level phenomena such as phase transitions. Using EDMD with stripe-shaped biphasic (SSBP) initial configurations and the Flyer-Target method, we analyze shock-induced effects near the crystal-fluid transition point. Packing fractions in the shocked region exceed the Alder transition point, with pressure overshoot due to compression-induced crystallization. Wavefront velocity increases with packing fraction in fluid and crystalline phases, but propagation delays occur in the coexistence regime. Cluster analysis reveals that crystal growth aligns with pre-existing cluster orientations and that initial positional disorder promotes multinuclear crystallization.

Diffusional characteristics and non-equilibrium phase transitions of active glass model in dense binary hard disk systems: The emerging field of “active glasses” explores the interplay between self-propulsion and glassy dynamics. We introduce Vicsek interactions into a binary hard disk glass-forming system and investigate diffusion and phase transitions via EDMD. A flocking transition is confirmed even at high densities. Near the transition, structural relaxation is enhanced, whereas in the ordered phase, diffusion slows despite

fluidization. The non-Gaussian parameter and four-point correlations exhibit two distinct peaks, suggesting a novel dynamic heterogeneity induced by Vicsek interactions.

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Generalizing bulk-edge correspondence to monitored quantum systems

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Quantum many-body systems subject to repeated measurements of local observables exhibit measurement-induced phase transitions (MIPTs) [1, 2]. A prominent example is the entanglement transition, where the steady-state entanglement entropy changes from a volume-law to an area-law scaling. Beyond these, MIPTs can also occur between distinct area-law phases characterized by the underlying topology of many-body states. In Ref. [3], we generalized the concept of bulk-edge correspondence, which has been established in equilibrium topological phases, to such monitored systems. This generalization is achieved by introducing an effective Hamiltonian derived from a quantum-trajectory evolution operator, which allows for the definition of an energy spectrum and a bulk topological invariant as a response to a symmetry twist. While this protocol was initially demonstrated for a monitored Kitaev-Majorana chain, it possesses the potential for application across diverse classes of measurement-induced topological phases.

In this project, we numerically investigated this protocol for two additional types of measurement-induced topological phases using the supercomputing facilities at ISSP (System B).

First, we considered a monitored version of the one-dimensional cluster state, which represents a symmetry-protected topological (SPT) phase protected by $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry. Our results show that the effective Hamiltonian exhibits a four-fold degeneracy in its energy spectrum under open boundary conditions. Fur-

thermore, we identified a quantized topological invariant by measuring a $\mathbb{Z}_2$ charge conditioned on the postselection of twisted measurement outcomes for the other $\mathbb{Z}_2$ charge. Numerical simulations confirmed that these signatures effectively identify phase transitions into either a trivial area-law phase or a volume-law entangled phase induced by unitary evolution.

Second, we examined a monitored version of the Su-Schrieffer-Heeger chain, an SPT phase protected by $U(1)$ and chiral symmetries. Similar to the monitored cluster state, we observed symmetry-protected zero modes within the bulk gap under open boundary conditions. We also computed a quantized topological invariant by generalizing the Zak phase to this monitored framework.

We are currently investigating the further extension of this protocol to a broader range of monitored SPT phases.

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A Microscopic Theory for Charge Imbalance in Nonequilibrium Superconductors

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In nonequilibrium electron systems, electron distributions generally deviate from the Fermi–Dirac function. However, a unified description of nonequilibrium electron distributions across different scattering regimes has remained challenging. To address this issue, we formulate a systematic approach based on the Keldysh Green’s function technique, in which scattering processes are incorporated self-consistently via self-energies [1]. We apply this framework to voltage-biased nanowires and demonstrate that it provides a unified description of nonequilibrium electron distributions over a wide range of transport regimes.

Using this framework, we further clarify the microscopic origin of charge imbalance in nonequilibrium superconductors [2]. Charge imbalance refers to a nonequilibrium state in which quasiparticles and Cooper pairs acquire distinct effective chemical potentials, and has traditionally been understood phenomenologically in terms of the branch-imbalance picture introduced by Tinkham. In the present work, we explicitly compute nonequilibrium electron distributions and show that voltage-induced asymmetric distributions naturally generate particle–hole imbalance, leading to charge imbalance. In this way, Tinkham’s branch-imbalance picture is microscopically justified in terms of the underlying nonequilibrium distribution function.

In these studies, the numerical calculations require self-consistent evaluation of Green’s functions with both frequency and internal

degrees of freedom, including iterative determination of scattering self-energies. Moreover, systematic exploration of parameter space, such as bias voltage and scattering strength, necessitates large-scale parallel computations. Therefore, the use of high-performance computing resources is essential to achieve tractable computation times.

The present study provides a unified understanding of nonequilibrium electron distributions and establishes a microscopic foundation for charge imbalance in superconductors. As a future direction, the framework developed here can be extended to time-dependent and periodically driven systems, opening the way to studies of the dynamical control of superconducting properties.

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Numerical study of the dynamical structure factor on the triangular-lattice Heisenberg antiferromagnet

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The coexistence of magnon excitations and spinon continuum in neutron scattering of magnetic materials has become an important topic in quantum spin system research [1], as evidenced by recent experiments with $\text{Ba}_3\text{CoSb}_2\text{O}_9$ and $\text{Cs}_2\text{Cu}_3\text{SnF}_{12}$ [2,3]. In this study, starting with the RPA approximation framework based on spinon operators (fermions) by Zhang and Li [4], we systematically investigated its validity and limitations through comparison with variational Monte Carlo methods and exact diagonalization that strictly incorporate constraints.

First, variational Monte Carlo calculations were performed for large-scale systems up to 900 sites using variational states derived from the spinon operator representation of the ground state of the triangular-lattice Heisenberg model. As a result, energy per site of $-0.5408(1)$ was obtained. Although this value is higher than $-0.5502(4)$ obtained by series expansion [5], it is lower than -0.538 obtained by spin wave calculations, confirming that it exhibits accuracy at or above that of conventional methods. On the other hand, in the calculation of the dynamic structure factor for a 36-site system, the result showed that the intensity of the continuity band was weak around point K and strong around point M, showing a trend opposite to that of the $\text{Ba}_3\text{CoSb}_2\text{O}_9$ experiment [2], similar to the RPA approximation [4].

To clarify the origin of this discrepancy, we compared in detail the variational states and exact diagonalization ground states for 36-site systems of square [1] and triangular lattices us-

ing spinon operators. The mean-field Hamiltonian H_{MF} includes only nearest-neighbor spinon hopping, and the states constructed from it correspond to nearest-neighbor RVB states. Furthermore, by introducing a staggered magnetic field H_{st} and constructing energy-optimized magnetic ordered states, we found that while the energy and static structure factors were reproduced relatively well, the overlap between the variational states and the exact ground state decreased rapidly with increasing system size. This result indicates that the nearest-neighbor valence bond alone cannot adequately represent long-range order, and that the introduction of long-range spinon hopping, i.e., long-range valence bonds, extending between different sublattices is essential.

Based on the above, we concluded that the construction of an extended H_{MF} including long-range hopping, and the systematic comparison of dynamic structure factors based on it using variational Monte Carlo and Lanczos methods, are critically important for improving the variational state that simultaneously describes RVB-like properties and magnetic order. This study provides a new perspective on understanding spinon continuum in two-dimensional quantum spin systems.

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Numerical study of magnon crystal states in a spin-1/2 distorted kagome antiferromagnet

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The magnetization plateaus $M/M_{\text{sat}} = 1/3$, $5/9$, and $7/9$ that appear in the magnetization process of kagome-lattice Heisenberg antiferromagnets have been thought to originate from the magnon crystal state (MCS), a triple degenerate state accompanied by spontaneous breaking of translational symmetry [1]. Using a model with a distortion corresponding to $\text{Y}_3\text{Cu}_9(\text{OH})_{19}\text{Cl}_8$, Bodaiji *et al.* studied a phase diagram on the distortion-magnetic field plane using the exact diagonalization method and identified six types of magnetization plateau phases [2]. Of these phases, the spin correlation function shows the same arrangement pattern as a single MCS, while the remaining three phases located on opposite sides of the distortion-zero line show a characteristic correlation pattern that extends throughout the entire lattice. However, the microscopic origin of this “lattice-extended” correlation has not been clear until now.

This study aims to provide a picture of this problem as a “quantum superposition of multiple degenerate MCSs.” Specifically, it focuses on the $M/M_{\text{sat}} = 7/9$ plateau, performs exact diagonalization on a 63-site system suitable for handling degeneracy [1], and constructs a variational framework by extracting a subspace spanned by only three MCSs as a low-energy effective space and solving the generalized eigenvalue problem within it. Under this setting, the wave function is expressed as a linear combination of the three MCSs, and by determining the optimal way in which each MCS component is superimposed, it becomes possible to directly track “what kind of MCS inter-

ference is producing the observed correlation pattern.”

This analysis revealed that, when the distortion vanishes, the phase switches via a first-order transition from a phase based on a single MCS to a phase based on a superposition state of two MCSs. Furthermore, in the limit of decreasing the distortion, we confirmed that the overlap between this variational state and the lowest energy state of exact diagonalization rapidly approaches 1, demonstrating that the essential physics near the $7/9$ plateau can be described solely by projection onto the MCS subspace and quantum hybridization within it. The spin correlation function calculated from the variational wavefunction and the exact ground state is quantitatively consistent, and in particular, it became clear that the correlation pattern extending across the entire lattice, as pointed out by Bodaiji *et al.*, can be naturally understood as an interference effect originating from the superposition of two MCSs. This study introduces a new theoretical framework for describing the magnetization plateau phase, shifting from a “single magnon crystal” to “quantum interference between multiple MCSs”, and represents an important step towards a unified understanding of the magnetism of strained kagome lattice systems.

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Vibration of Granular System: Relation Between Viscoelastic Relaxation and Particle Dynamics

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Understanding the rheological response of granular materials to mechanical perturbations is of broad importance across disciplines ranging from earth science to chemical engineering. This study concerns the rheology of granular materials under external perturbations. In the course of this research, an unexpected but significant finding was obtained regarding the mechanical response of granular materials to small-amplitude perturbations [1]. In addition, related results were obtained on the rheological behavior of structured granular materials [2, 3].

The main part of this study was carried out theoretically. Numerical simulations using the discrete element method (DEM) implemented in LAMMPS were performed to support the theoretical analysis, including preliminary explorations of parameter space and numerical checks of the stress-strain relation up to yielding. These simulations were performed on the i8cpu and F1cpu partitions of the System B supercomputer (Ohtaka), typically on a single node.

As a model system, we considered a granular assembly arranged in a two-dimensional triangular crystalline configuration under uniform shear. The theoretical analysis focused on the stress-strain relation near yielding, the dispersion relation $\omega(k)$, and the vibrational density of states (vDOS), which characterizes the vibrational spectrum of the system. The DEM calculations were used to examine the consistency of the predicted yield stress and yield

strain.

A central result is that, near the yielding strain, many k -points within a single vibrational branch soften simultaneously, forming a cross-shaped soft region in wave vector space. This softening over an extended region of wave vector space contrasts sharply with the behavior of amorphous solids, where only spatially localized vibrational modes become unstable near yielding. This multimode softening in our system is directly reflected in the vibrational spectrum: at small shear strains, the system exhibits a linear dispersion relation $\omega \sim k$, consistent with the continuum wave equation, whereas near the yielding strain a large number of low-frequency modes are excited and the dispersion relation crosses over to a quadratic form $\omega \sim k^2$. Correspondingly, the vDOS crosses over from the Debye law $D(\omega) \sim \omega$ to an anomalous scaling $D(\omega) \sim \omega^{1/2}$. These scalings were also derived explicitly and reveal an essential difference in the yielding mechanism between crystalline and amorphous granular systems. We validated the theoretical framework by comparing the theoretically predicted yield stress and yield strain against the DEM simulation results.

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Role of counterions in the ion-mediated permeation of hydrophobic ions into lipid bilayers

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The lipid bilayer, which constitutes the basic structure of the cell membrane, exhibits selective permeability. For example, sodium ions are transported across the membrane through specific ion channels. In general, because ions carry electric charges, they cannot pass through the hydrophobic core of the lipid bilayer, and therefore mechanisms such as ion channels are considered necessary for their transmembrane transport.

However, there are ionic species that are capable of directly permeating lipid membranes, although the mechanisms underlying this process remain poorly understood. For example, it is known that direct membrane permeation of ionic compounds is promoted when their counterions are more hydrophobic [1]; however, this phenomenon cannot be explained by classical partitioning models.

In this study, we aim to perform free-energy calculations of the membrane permeation of hydrophobic ions using an all-atom model to elucidate the role of counterions. Clarifying the mechanisms of ionic compound permeation across lipid membranes is essential for the advancement of applied research, such as the transport of ionic drugs using phospholipid vesicles.

To elucidate the effect of counterions on the membrane permeation of the hydrophobic ion R6G^+ , we calculate the free energy profile of R6G^+ using the hydrophilic chloride ion and the hydrophobic perchlorate ion as counter-

ions. We employed the umbrella sampling, and approximately 20 independent simulations were performed from within the membrane to the aqueous phase.

After 50 ns of equilibration for each window, a 50 ns production run was carried out. The CHARMM36 force field was used for DOPC lipids [2, 3] and TIP3P-CHARMM [4] was applied for water. The force fields for R6G^+ and the perchlorate ion were derived from Refs. [5] and [6], respectively. Molecular dynamics (MD) simulations were performed with NAMD and the free-energy profile was calculated using the Grossfield's WHAM code [7].

The calculated free energy profiles are shown in Figure 1. For both counterions, chloride and perchlorate, R6G^+ is most stabilized near the membrane interface. The system containing chloride ions exhibits a smaller energy barrier for entering the membrane and higher stability within the membrane, suggesting that R6G^+ can more readily permeate the membrane in the presence of chloride ions.

However, this result is contrary to experimental observations. Electrochemical measurements using DOPC vesicles indicate that R6G^+ permeates the membrane more easily when perchlorate ions are present as counterions [1]. The origin of this discrepancy will be investigated in future studies.

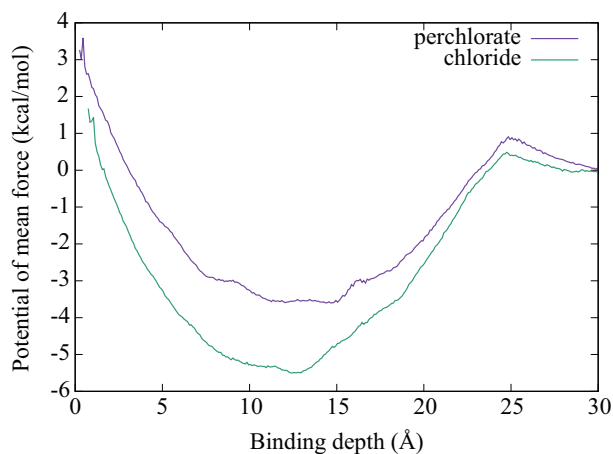


Figure 1: Free energy profiles of $R6G^+$ in the presence of chloride or perchlorate ions.

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Numerical Study of Pipe Flow and Clogging of Cells

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Collective cell migration is a phenomenon, which spontaneously delivers cells to proper positions, where the cells function. Collective migration helps our understanding of active matter by providing a typical example of its collective behavior. In contrast to simple active matter, the mechanism that stabilizes collective cell migration remains elusive in many physical aspects owing to its complexity. To overcome the complexity, the virtual experiment, using numerical simulations based on theoretical models, has been a standard method for clarifying the stabilization mechanism, in order to support its experimental clarification, which often encounters difficulties in the necessary controls over cell features.

In this work, we apply a theoretical model to examine guiding scaffolds of cell migration. Guiding scaffolds are well known as a stabilizing origin for the migration of neurons, both in artificial experiments and in physiological environments [1, 2]. The scaffold chemically guides migration along the shortest path to the appropriate positions. The physical mechanism of this stabilization is not well understood from a physics point of view, and its clarification may provide fundamental insights that help us develop a treatment for neuron dysfunction. Based on numerical simulations using a theoretical model, we investigate the effect of scaffold-guided collective cell migration in tissues and examine it as a treatment for dysfunction in collective migration.

Migration dysfunction results from various mechanisms, including disorders of intercellular interactions. One significant interaction

contributing to the disorder is overstrengthened cell-cell adhesion, which promotes cell aggregation in certain cases [3]. This cell aggregation inhibits collective cell migration. The guiding scaffold may lead to a transition from cell aggregation without migration. We model this type of cell aggregation and examine the effect of guiding scaffolds on cell aggregation to stabilize collective cell migration [4].

Our results show that the guiding scaffold can induce a transition from cell aggregation to collective migration as follows. The collective migration is absent under low-strength scaffold guidance. At a certain strength of guidance, the collective velocity of cells starts to increase linearly. With a further increase in guidance strength, the collective velocity disappears. Therefore, collective migration occurs in an optimal range of guidance strength.

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Phonon-mediated Chirality Control in Molecular Triangles by Photoirradiation

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We have studied the ultrafast quantum dynamics of a triangular molecular system in which Frenkel excitons are coupled to local optical phonons [1]. The purpose of this project was to clarify how phonon degrees of freedom mediate the control of exciton chirality under photoirradiation. Numerical calculations were performed using the facilities of the Supercomputer Center, Institute for Solid State Physics, The University of Tokyo.

We considered a minimal three-site exciton–phonon model. Each molecular site was described as a two-level excitonic system represented by a pseudospin, and each exciton was locally coupled to an Einstein phonon. The exciton chirality was defined by the scalar spin chirality of the pseudospin variables. By introducing a symmetry-adapted phonon basis for the threefold rotational symmetry of the triangle, we separated the phonon modes into a totally symmetric mode and two nontrivial symmetry modes. The latter modes form composite exciton–phonon states that directly control the expectation value of the chirality operator.

Using numerical diagonalization, we first

analyzed the eigenstates of the exciton–phonon Hamiltonian. The results show that the chirality is strongly correlated with the occupation of the symmetry-adapted phonon modes. In particular, phonon excitations in the nontrivial symmetry sector give rise to discrete changes in the chirality expectation value. This provides a microscopic mechanism by which phonons can act as active quantum degrees of freedom for controlling molecular chirality, rather than merely as an environment causing decoherence.

We then investigated real-time dynamics under semiclassical photoirradiation by solving the time-dependent Schrödinger equation. Starting from the ground state of the exciton–phonon system, we examined how the chirality evolves after optical excitation. We found that photoirradiation can induce a sign change of the exciton chirality when the excitation frequency is tuned to an appropriate absorption peak. This chirality inversion is caused by the competition between electronic transitions and phonon generation driven by exciton–phonon coupling. The light intensity plays an important role: moderate intensity allows phonon-assisted chirality inversion, whereas excessively strong

fields lead to rapid Rabi oscillations that suppress the phonon adjustment required for efficient control.

We also calculated the circular dichroism response of the triangular exciton–phonon system. The results indicate that the sign of the circular dichroism signal reflects the sign of the exciton chirality, suggesting that the chirality inversion may be detected through polarization-dependent optical measurements.

These results demonstrate that coherent

phonon dynamics can provide a route to controlling chiral excitonic states in triangular molecular systems. The present study gives a theoretical basis for phonon-mediated chirality control and may be extended to more general light–matter systems, including cavity-coupled exciton–phonon–photon states.

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Numerical Study of One Dimensional Frustrated Quantum Spin Systems

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1 Model

We investigate the ground-state phases of $(1/2, 1/2, 1)$ mixed diamond chains with single-site anisotropy described by the following Hamiltonian:[1]

$$\mathcal{H} = \sum_{l=1}^L \left[(1 + \delta) \mathbf{S}_l (\boldsymbol{\tau}_l^{(1)} + \boldsymbol{\tau}_{l-1}^{(1)}) + (1 - \delta) \mathbf{S}_l (\boldsymbol{\tau}_l^{(2)} + \boldsymbol{\tau}_{l-1}^{(2)}) + \lambda \boldsymbol{\tau}_l^{(1)} \boldsymbol{\tau}_l^{(2)} + D \tau_l^{(2)z2} \right], \quad (1)$$

where $\mathbf{S}_l, \boldsymbol{\tau}_l^{(1)}$ and $\boldsymbol{\tau}_l^{(2)}$ are spin operators with magnitudes $S_l = \tau_l^{(1)} = 1/2$ and $\tau_l^{(2)} = 1$, respectively. The number of unit cells is denoted by L . The spontaneous magnetization M_{sp}^z in the ground state is defined by

$$M_{\text{sp}}^z = \left\langle \sum_{l=1}^L \left[S_l^z + \tau_l^{(1)z} + \tau_l^{(2)z} \right] \right\rangle, \quad (2)$$

where $\langle \rangle$ denotes the expectation value in the ground state.

The lattice structure is depicted in Fig.1. We consider the region $\lambda \geq 0$ and $-1 \leq \delta \leq 1$. The isotropic case ($D = 0$) is investigated in [2, 3].

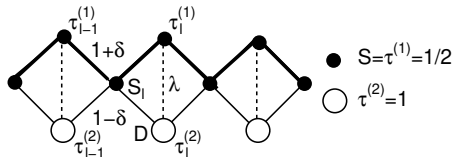


Figure 1: Structure of the diamond chain investigated in this work.

2 Numerical Results

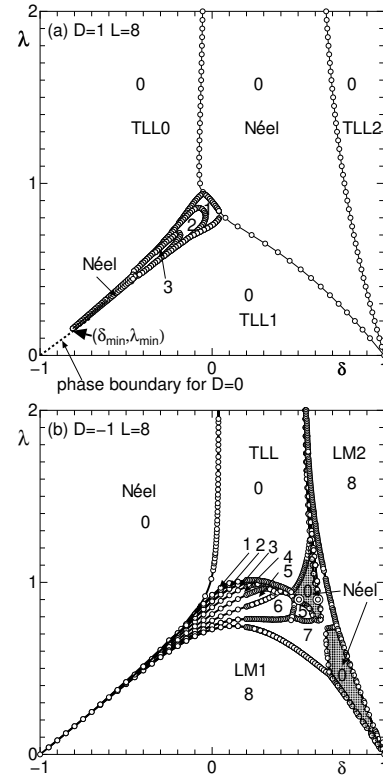


Figure 2: Ground-state phase diagrams based on the NED data with $L = 8$ for (a) $D = 1$ and (b) $D = -1$. The number indicated for each phase is M_{sp}^z . The double circles ($\odot$) in (b) are the phase boundaries obtained by DMRG with $L = 48$.

We have carried out the numerical exact diagonalization (NED) calculation for $L = 4, 6$, and 8 . The phase diagrams for $L = 8$ are shown in Fig.2 for (a) $D = 1$ and (b) $D = -1$.

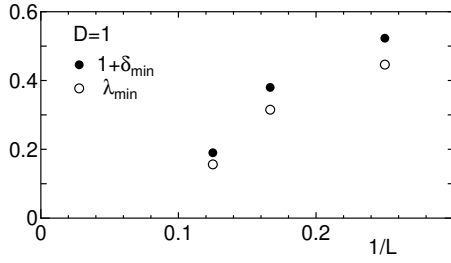


Figure 3: Minimum value of $1+\delta$ and λ plotted against $1/L$ in the narrow Néel phase for $D = 1$.

The number indicated for each phase is M_{sp}^z of the ground state. For $D = 1$, three kinds of Tomonaga-Luttinger liquid phases (TLL0, TLL1, TLL2) are found in addition to the Néel phase, and partial ferrimagnetic (PF) phases. The end point $(\delta_{\text{min}}, \lambda_{\text{min}})$ of the narrow Néel phase between TLL0 and TLL1 phases tends to $(\delta_{\text{min}}, \lambda_{\text{min}}) = (-1, 0)$ in the thermodynamic limit as shown Fig.3 confirming that TLL0 and TLL2 phases are different phases. The phase boundary between the TLL0 and TLL1 phases is close to the TLL-LM1 phase boundary for $D = 0$ shown by the dotted line in Fig.2(a). Hence, this phase boundary is insensitive to the value of D . It should be remarked that the Néel phase is present even in the case of easy-plane anisotropy $D > 0$. This is an example of the anisotropy inversion phenomena previously reported in frustrated spin-1/2 chains with trimer structure[5]. For $D = -1$, two kinds of Lieb-Mattis type ferrimagnetic phases[4] (LM1, LM2) appear in addition to the Néel, TLL and PF phases. According to the DMRG calculation for $L = 48$ shown by $\odot$ in Fig.2(b), the upper shaded part of the Néel phase remains in the thermodynamic limit, while the lower shaded part vanishes in the thermodynamic limit. We expect that the latter region will be replaced by the PF phase with $0 < m_{\text{sp}} < 1$ as in the isotropic case.[3] The anisotropy inversion phenomenon is also observed for large λ region where the TLL phase remains even in the presence of easy-axis anisotropy $D < 0$.

The numerical diagonalization program is based on the TITPACK ver.2 coded by H. Nishimori.

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Scrambling in long-range interacting quantum systems

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Out-of-time-order correlator (OTOC) has attracted attention in non-equilibrium statistical mechanics, quantum information, and quantum gravity. The time evolution of the OTOC estimates the scrambling time t_* when local perturbation propagates to the entire system. Estimating the scrambling time in long-range interacting quantum spin systems, where the interaction decays as a power law $J \sim r^{-\alpha}$ with distance r , is still challenging on both theoretical and numerical sides.

Here, we propose a discrete truncated Wigner approximation (DTWA) based method for computing temporal correlation functions including OTOCs. The DTWA method needs a computational cost of the order of N^2 , where N is the system size, whereas exact methods generally require exponentially growing computational costs. Thus, DTWA offers a promising approach for exploring dynamical features of large-sized systems even when $\alpha > 0$. The method is applied to calculate an auto-correlation function, a squared commutator of local operators, and its higher-order extensions, and compared between systems with varying values of α . Our numerical results reproduce the exact dynamics for the average spreading of quantum information (i.e., squared commutators) across all time regimes for $\alpha \leq d$. Furthermore, we identify the limitations of the DTWA method when simulating scrambling dynamics for $\alpha > d$ and the fastest spreading of quantum information. Finally, we apply the

DTWA method to investigate N dependence of t_* for $\alpha \leq 1$ on a one-dimensional lattice and compare the numerical result with a theoretical lower bound. Figure 1 reveals that the scaling behavior of t_* for large systems changes depending on the value of α .

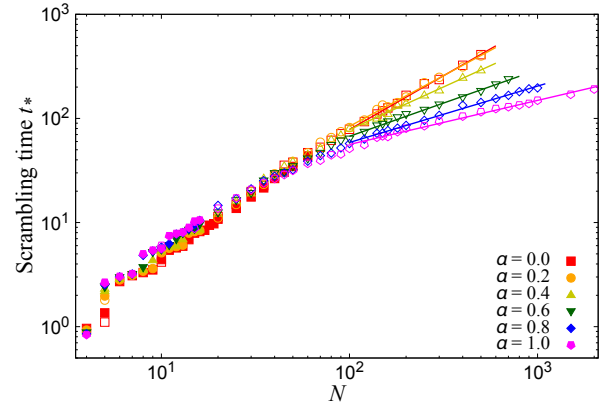


Figure 1: System-size dependence of the scrambling time t_* for different values of α . Open symbols and filled symbols indicate the DTWA results and the exact results, respectively. The bold lines are fitting using data of $N \geq 100$.

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Theoretical study for excited states of firefly bioluminescence emitters

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Analogues of firefly bioluminescent substrates are attracting attention as next-generation luminescent probes for *in vivo* imaging techniques for animal tissues and cells, and their development is currently underway [1]. As such substrate analogues, not only AkaLumine, of which bioluminescence color is red (675 nm), but also more water-soluble analogue seMpai producing similar bioluminescence color have been reported [2]. To investigate the differences in the electronic states of these analogues, we performed optimization of structure and vibrational analysis of the ground states for their oxy-form using the density functional theory (DFT) method. We also determined the structures of the excited states using the time-dependent (TD) DFT method.

Since the chemical species studied in this research consist of approximately 30 atoms, the computational time for preliminary calculations using a small number of basis sets, as well as for structural optimization and vibrational analysis in the ground state, was less than 24 hours. Therefore, we primarily used the F1cpu on System B for these calculations. On the other hand, since computational jobs involving structural optimization of excited states take more than one day to complete, we primarily used the L1cpu on System B.

Based on preliminary calculation results for the oxy-form of AkaLumine, we performed the quantum chemical calculations using Conductor-like Polarizable Continuum Model (CPCM) and Solvation Model based on Den-

sity (SMD) for the solvent effects. We found that, in the case of oxy-AkaLumine, structural optimization calculations using SMD failed to converge. Since the same problem occurred even in calculations with improved integration accuracy, this would be due to noise in the SMD method in Gaussian16, rather than an issue with the installation process or system B of Super Computer Center in ISSP.

According to the results of structural optimization, absorption calculations, and relative concentration analyses in 2024 for the conjugate acids and bases of seMpai, which were presumed to exist in aqueous solution, it was found that the chemical form of seMpai at pH 8, at which bioluminescence spectra is measured, is a carboxylate anion structure like that of AkaLumine [3, 4]. Following these results, the structures of oxy-AkaLumine and oxy-seMpai were determined. The results revealed that the charge distributions of the Highest Occupied Molecular Orbital (HOMO) for oxy-AkaLumine and oxy-seMpai are very similar to each other. Those of the Lowest Unoccupied Molecular Orbital (LUMO) are also similar to each other. The main configuration of the first excited states for all chemical species was the excitation from HOMO to LUMO.

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Vortex structures and superconducting properties in quasicrystals

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We have investigated superconducting properties of quasiperiodic systems using large-scale numerical simulations based on the Bogoliubov–de Gennes (BdG) mean-field theory. In particular, we studied vortex states and the orbital upper critical field $B_{c2}(T)$ in an s -wave superconductor defined on the Ammann–Beenker tiling with octagonal symmetry.

Although previous studies have addressed intrinsic pinning of a single vortex [1] and spatially inhomogeneous superconducting states [2], the collective organization of vortices under strong magnetic fields and its impact on $B_{c2}(T)$ remain unclear. In quasiperiodic systems, intrinsic spatial inhomogeneity of the order parameter suggests that vortices preferentially penetrate weakly superconducting regions, which can significantly modify vortex configurations and field responses. Clarifying these effects is particularly relevant in light of recent experimental studies on magnetic-field responses in quasicrystalline superconductors [3].

Due to the absence of translational symmetry, the BdG equations must be solved in real space for large system sizes, leading to a substantial computational cost. The supercomputer system enabled us to perform calculations for systems with sizes up to $\mathcal{O}(10^3)$ sites, including diagonalization of large sparse matrices and extensive parameter sweeps over temperature and magnetic field.

We find that vortex configurations in

quasiperiodic systems differ qualitatively from the Abrikosov triangular lattice observed in periodic superconductors. Near half filling, vortices form patterns reflecting the underlying eightfold symmetry. Furthermore, vortices preferentially occupy weak-pairing regions, resulting in vortex clustering and the formation of giant vortex states. This effect effectively protects strongly superconducting regions from orbital pair breaking.

As a consequence, the orbital upper critical field $B_{c2}(T)$ is significantly enhanced compared to periodic systems. In addition, $B_{c2}(T)$ exhibits anomalous low-temperature behavior, showing an approximately linear increase down to low temperatures without clear saturation.

A manuscript based on these results is currently under preparation [4].

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Spontaneous formation of multiple-Q orders in two-dimensional Hubbard models

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In recent years, the multiple-Q orders in magnetic systems have attracted attention because they sometimes reveal nontrivial magnetic structures such as magnetic skyrmions. These structures are realized in both non-centrosymmetric and centrosymmetric systems. In noncentrosymmetric systems, the competition among the Dzyaloshinskii-Moriya (DM) and ferromagnetic interactions causes the multiple-Q orders. In the case of centrosymmetric systems, the formation mechanism of nontrivial multiple-Q orders is not unique and still under investigation [1, 2].

The purpose of the present research is to investigate the multiple-Q orders in the centrosymmetric systems, starting from the itinerant electron model where the electronic structures play an important role in forming the multiple-Q orders. Specifically, we investigate the multiple-Q orders in the centrosymmetric triangular-lattice single-band Hubbard model by means of the molecular spin dynamics (MSD) method [3]. The present formulation of the MSD adopts the static approximation to the functional integral method and the isothermal molecular dynamics technique, and reduces to the generalized Hartree-Fock approximation at the ground state.

Starting from a random distribution of local magnetic moments, the MSD scheme can automatically determine the stable magnetic structure. In this scheme, the most time-consuming process is the magnetic force calculation at each time step, where the local elec-

tronic structures are calculated in real space by means of the recursion method. We have adopted the MPI parallel calculation scheme in the recursion calculation and found it effective in saving both computing time and CPU resources.

In the present work, we have included the 1st, 2nd and 3rd neighbor transfer integrals t_i ($i = 1, 2, 3$) in the Hubbard model. We have performed magnetic structure calculations on a hexagonal supercell with 972 lattice points, which is embedded in a large cluster consisting of 6 such supercells, each of which are connected by the periodic boundary condition. Under zero magnetic field and the fixed value of the temperature $T/t = 0.0005$, we have explored the magnetic structures changing the Coulomb interaction strength U/t_1 , transfer integral ratios t_2/t_1 , t_3/t_1 and the electron number n .

In the case of $t_2 = 0$, $t_3/t_1 = -0.42 \sim -0.40$, $3Q + 1Q$ order is stabilized for $U/t_1 = 7.0$ and $n = 1.20 \sim 1.22$, where the magnetic structure shows phase separation. The electronic density of states becomes zero in the vicinity of the Fermi energy E_F , opening a gap at E_F .

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Understanding the characteristics of sentence production based on differences in language acquisition methods

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Language has been attracted the interests of researchers in the field of physics (e.g., [1, 2, 3]). However, grammar for natural language has not been considered there. We employ the combinatory categorial grammar (CCG) to deal with natural languages mathematically. The definition of CCG is as follows. First, we define noun (N), noun phrase (NP), and sentence (S) as ground category. We then employ operators / and \. These operators represent the grammar. Let us consider two categories A and B. The category A/B indicates that if the category B emerges after this category, the categories are merged into the category A. The category A\B indicates that if the category B emerges before this category, the categories are merged into the category A. If we write the sequence of the categories A and B as A+B, these rules are described with the equations

$$A/B + B \rightarrow A, \quad (1)$$

$$B + A\backslash B \rightarrow A. \quad (2)$$

Equations (1) and (2) are called forward and backward functional application rules, respectively. For example, let us write intransitive verb with CCG for English. If the noun phrase comes before the intransitive verb, the sentence is generated. We therefore conclude that the intransitive verb is a category $S\backslash NP$. An additional example is the adjective. In languages like English where modifiers precede

the modified word, it can be written as N/N with CCG. Notably, the operators can be utilized recursively. With this framework, all categories are represented by the combinations of N, NP, S, /, and \. The categories other than the ground categories such as intransitive verb $S\backslash NP$ are called syntactic categories.

We regard the sentence as the sequence of the categories, and apply the metropolis method to CCG. As an initial condition, the first step is to arrange the categories randomly. We then select one of the categories and change it into another category (i.e., upgrade). If the sequence from the beginning of the sentence to the selected category is grammatical, we accept the upgrade. On the other hand, if the sequence is not grammatical, we accept it with probability $\exp(-\Delta E/k_B T)$, where ΔE is the measure of instability of the sequence, k_B is the Boltzmann constant, and T is temperature. We assume the scale unit where $\Delta E/k_B$ is normalized to be unity. Temperature can be interpreted as the disturbance for the grammar, and describes how the learner is familiar with the grammar.

We consider the generating mechanism of the sentence with N_W words. We fix $N_W = 40$ in the current study. Though we initially arrange categories randomly, as mentioned above, note that the first category is fixed to be an article. We then apply the metropolis method. We repeat the calculation 10000 times for each temperature. We inves-

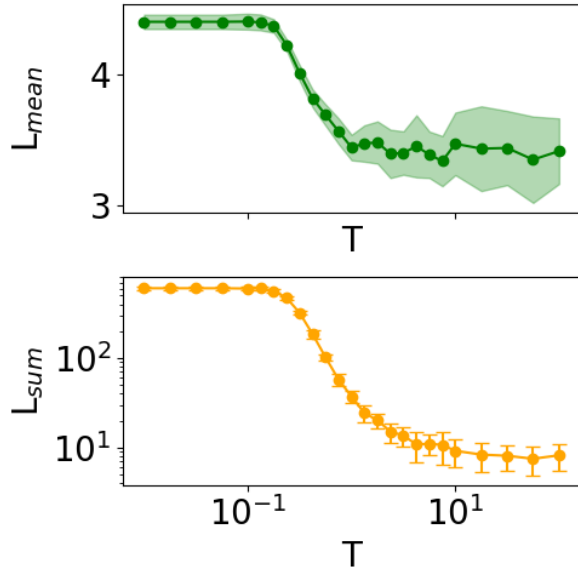


Figure 1: Dependences of L_{mean} and L_{sum} on T [4].

investigate the probability that the grammatically correct sentences are generated. Using the probability, we calculate the expected value of the sentence length L , L_{mean} . We also investigate numbers of the grammatically-finished sentences, L_{sum} , for each temperature.

The upper panel in Fig. 1 describes the relationship between T and L_{mean} . Discontinuous behavior of dependence of L_{mean} on temperature is observed; above a certain temperature, correct sentences are hardly generated anymore. The boundary is $T \sim 0.1$. We can observe that L_{sum} also shows phase-transition-like behavior (lower panel in Fig. 1). The probability generating grammatically correct sentence is almost 5 – 6% for $T < 0.1$, whereas it is almost 0.05% for $T > 1$.

High temperature represents the children who do not understand the grammar completely. The language acquisition may be a phase-transition process.

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Molecular dynamics simulation of graphene-nanosapcer stacking heterostructure properties

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In our previous studies, we investigated graphene (Gr) stacking structures containing nanodiamond (ND) nanopacers and carbon nanotube (CNT) spacers. These studies showed that the insertion of nanopacers between Gr layers effectively modulates the interlayer distance and interlayer interaction of multilayer Gr [1,2]. Building on these studies, this year we investigated the loading–unloading behavior of graphene–carbon nanotube (Gr–CNT) hybrid systems using molecular dynamics (MD) simulations and nanoindentation experiments.

MD simulations were conducted using the open-source software LAMMPS. The AIREBO potential was used to describe short-range carbon–carbon interactions, while the LJ potential was employed for interlayer van der Waals interactions. Dynamic relaxation was performed using the velocity-Verlet algorithm to obtain energy-minimized structures.

The MD simulations focused on stacked Gr–CNT structures, in which CNTs were confined between two graphene layers. By applying periodic boundary conditions, we examined systems with different intertube spacings, CNT diameters, and wall numbers.

Representative snapshots of the MD simulations under different structural conditions are shown in Figure 1.

Under certain conditions, the Gr–CNT structures exhibited mechanical bistability with two stable configurations: adhesion and separation of the graphene layers. This bistability originates from the competition between interlayer van der Waals attraction and elastic deformation of the graphene layers and CNTs. The simulated loading–unloading curves showed clear hysteresis, indicating energy dissipation associated with structural transitions between stable configurations.

To experimentally verify the mechanical behavior predicted by the simulations, reduced graphene oxide–carbon nanotube (rGO–CNT) hybrid films were fabricated as macroscopic assemblies corresponding to the unit structures modeled in the MD simulations. Atomic force microscopy-based nanoindentation measurements were performed on the rGO–CNT films. The obtained force–displacement curves exhibited pronounced hysteresis and larger dissipation energy compared with pure rGO films, in good agreement with the

simulation results.

These results show that the mechanical response of Gr–CNT hybrid systems is governed by the balance between van der Waals interactions and elastic deformation. The combined MD simulation and nanoindentation approach provides fundamental insight into the design of graphene-based hybrid microstructures with tunable mechanical stability, hysteresis, and energy dissipation properties. The outcomes of this study have been compiled into a manuscript and submitted for publication [3].

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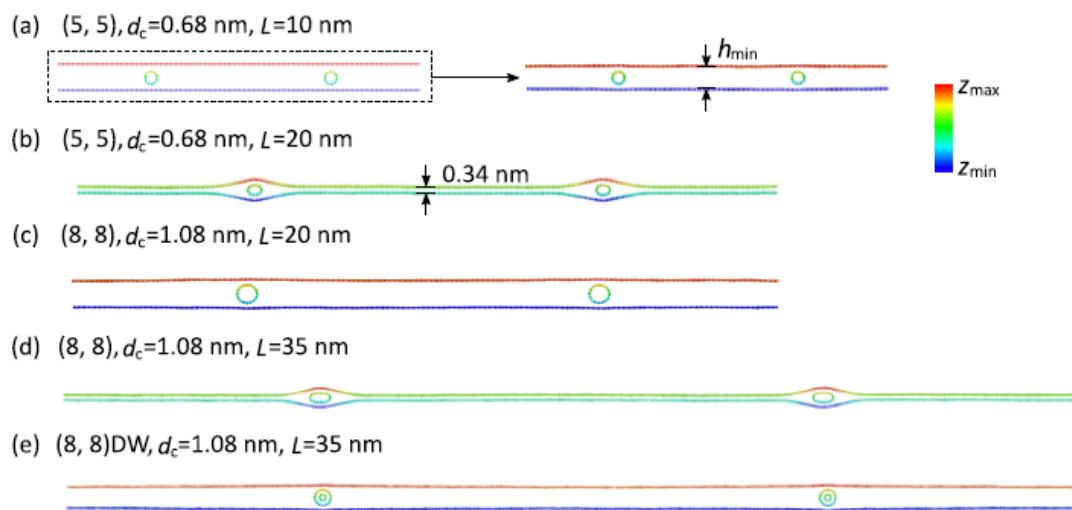


Fig. 1 (a) Relaxed configurations obtained from MD simulations of the Gr–CNT stacked structure with different intertube distances L , CNT diameters d_c , and wall numbers.