物性研究所セミナー

標題：軟 X 線吸収分光のすすめ
日時：2023 年 12 月 18 日(月) 午後 1 時～
場所：6 階大講義室＆Online
講師：新部 正人
所属：物性研究所　松田巌研究室
要旨：

軟 X 線吸収分光(SXAS)は、放射光分光ビームラインにおいて試料とピコアンメータがあれば出来る簡便な分光分析手法であるが、元素分析、状態分析、分子結合性評価、結晶配向性評価など様々な分析評価ができる。本講演では、筆者が行った、あまり知られていない軟 X 線分光実験を紹介することにより、軟 X 線吸収分光法を理解して頂くための、主に初学者向けのお話をされた。

内容は、軟 X 線吸収分光の定量性評価、全電子収量(TEY)法と全蛍光収量(法での検出深さの評価とその応用、h BN 薄膜における複数 π ピークの同定、薄膜結晶成長の in situ 観測への応用、He path を用いた大気圧下軟 X 線吸収分光法の開発、吸収分光と発光分光の組み合わせで見えるもの、などである。

標題：電場と温度勾配による非線形 Hall 効果の微視的理論
日時：2023 年 12 月 22 日(金) 午後 4 時～午後 5 時
場所：物性研究所 6 階第 5 セミナー室（A615）**及び** Online（Hybrid）
講師：山口 皓史
所属：理化学研究所 CEMS
要旨：

外場に対し非線形に応答する非線形輸送現象が近年注目を集めている。非線形輸送現象は線形応答に対する補正項であるばかりではなく、本質的に異なる現象を引き起こすこともでき、実際に非線形 Hall 効果や電流の非相反伝搬、非線形光学効果といった非線形特有の現象が多く知られている。本研究では特に電場と温度勾配を互いに垂直に印加した場合に、両者の外積に比例する電流が生じる効果（非線形カイラル熱電気(Nonlinear Chiral Thermo-Electric, NCTE) Hall 効果と呼ぶ）に着目する。NCTE Hall 効果は Weyl 粒子系において生じることが報告され[1]、その後半古典論に基づいた解析[2,3]から固体中でも生じうることが指摘された。一方で、具体的な固体のモデルで生じることを示した例はなく、また一般のバンド構造に対する微視的な定式化も不十分となっている。

本発表では、一般のバンド構造に対する NCTE Hall 効果を微視的に定式化し、具体的なモデルにおいてそれが発現することを示す[4]。非平衡（Keldysh）Green 関数を用いて電場と温度勾配の非線形応答を取り扱い、NCTE Hall 効果を定式化する。得られた表式をバンド表示することで、先行研究では現れなかった寄与があることを見る。また、NCTE Hall 効果が生じる簡単なモデルと、カイラル結晶の具体的な強束縛モデルにおいて、実際に NCTE Hall 効果が生じることを示す。

[1] Y. Hidaka, S. Pu, and D.-L. Yang, Phys. Rev. D 97, 016004 (2018).
[2] R. Nakai and N. Nagaosa, Phys. Rev. B: Condens. Matter Mater. Phys. 99, 115201 (2019).
[3] R. Toshio, K. Takasan, and N. Kawakami, Phys. Rev. Res. 2, 032021 (2020).
[4] T. Yamaguchi, K. Nakazawa, and A. Yamakage, arXiv:2305.05273 (2023).

標題： Magnetization and Polarization Switching in a Family of Heterometallic Complexes with Electron Transfer and Spin Transition Behavior
日時： 2023 年 12 月 22 日(金) 午前 11 時～午後 0 時
場所： Online
講師： Shu-Qi Wu 助教
所属： 九州大学
要旨：

Spin transition behavior in molecular crystals has attracted wide attention in the field of molecular physics and chemistry. By appropriate chemical design, the transition properties (e.g. transition temperature) could be finely tuned. In this talk, we will discuss about the electron dynamics in two systems, i.e. [(Fe(RR-cth))(M(SS-cth))(μ-dhbq)]X 3 and [(Co(RR-cth))(M(SS-cth))(μ-dhbq)]X 3 crystallized in the P2 1 space group (cth = 5,5,7,12,12,14-hexamethyl-1,4,8,11-tetraazacyclotetradecane, H 2 dhbq = 2,5-dihydroxy-1,4-benzoquinone, M = Co, Cr and Ga, X = PF 6 − and AsF 6 −). The former family exhibits a transition process at Fe site with thermally hysteretic behavior, followed by a gradual electron transfer between the Fe and ligand sites. Owing to the asymmetrical changes in the molecular structures and changes in metal-ligand covalency, a substantial polarization change has been observed. Furthermore, these compounds undergo similar processes when subjected to pulsed magnetic fields at lower temperatures, resulting in a comparable polarization change. The latter family exhibits an electron transfer coupled spin transition process at Co site, which leads to a polarization change as large as 2~3 μC/cm 2 . Interestingly, by trapping the electron-transferred metastable state at low-temperatures, a persistent light-induced polarization change could be observed.

標題： 高次高調波に着目した非摂動論的な領域における非線形光学の展望
日時： 2023 年 12 月 22 日(金) 午後 1 時～午後 2 時
場所： 物性研究所本館 6 階 第 5 セミナー室 (A615)
講師： 玉谷 知裕
所属： 東京大学物性研究所
要旨：

近年高強度テラヘルツ光源開発の進展に伴い、半導体などの固体において非摂動論的な非線形光学現象が観測されるようになった。これらの現象を理解するためには、これまでの摂動論的なアプローチを超えて非摂動論的な領域にまで非線形光学という学問分野を拡張する必要がある。そこで本講演では特に高次高調波発生に焦点を当て、この現象を非摂動論的領域に拡張する際の考え方を示すと共に、理論と実験の比較を行う。そしてこの考え方を用いて非摂動論的な非線形光学現象の制御法についての議論を行う。

標題： The Self-Learning Monte Carlo Method: Accelerating Simulations with Machine Learning
日時： 2023 年 12 月 26 日(火) 午後 1 時～午後 2 時
場所： 物性研究所本館 6 階 第 4 セミナー室 (A614)
講師： Yuki Nagai
所属： Japan Atomic Energy Agency
要旨：

We have introduced a general method, dubbed self-learning Monte Carlo (SLMC), which speeds up the MC simulation by designing and training a model to propose efficient global updates. We have developed the SLMC in various kinds of systems for electrons[1], spins[2], atoms[3], and quarks and gluons[4].

For example, we proposed an efficient approach called self-learning hybrid Monte Carlo (SLHMC) method, which is a general method to make use of machine learning (ML) potentials to accelerate the statistical sampling of first principles density-functional-theory (DFT) simulations[3]. In the SLHMC simulation, the statistical ensemble is sampled exactly at the DFT level for a given thermodynamic condition. Meanwhile, the ML potential is improved on the fly by training to enhance the sampling, whereby the training dataset, which is sampled from the exact ensemble, is created automatically.

In this talk, I will show the basic concept of SLMC and various kinds of applications.

[1] YN, H. Shen, Y. Qi, J. Liu, and L. Fu, Self-Learning Monte Carlo Method: Continuous-Time Algorithm, Phys. Rev. B 96, 161102 (2017).; YN, M. Okumura, K. Kobayashi, and M. Shiga, Self-Learning Hybrid Monte Carlo: A First-Principles Approach, Phys. Rev. B 102, 041124 (2020).

[2] H. Kohshiro and YN, Effective Ruderman–Kittel–Kasuya–Yosida-like Interaction in Diluted Double-Exchange Model: Self-Learning Monte Carlo Approach, J. Phys. Soc. Jpn. 90, 034711 (2021).;YN and A. Tomiya, Self-Learning Monte Carlo with Equivariant Transformer, http://arxiv.org/abs/2306.11527.

[3] YN, M. Okumura, K. Kobayashi, and M. Shiga, Self-Learning Hybrid Monte Carlo: A First-Principles Approach, Phys. Rev. B 102, 041124 (2020).;K. Kobayashi, YN, M. Itakura, and M. Shiga, Self-Learning Hybrid Monte Carlo Method for Isothermal-Isobaric Ensemble: Application to Liquid Silica, J. Chem. Phys. 155, 034106 (2021).

[4] YN, A. Tanaka, and A. Tomiya, Self-Learning Monte Carlo for Non-Abelian Gauge Theory with Dynamical Fermions, Phys. Rev. D (2023).;Y. Nagai and A. Tomiya, Gauge Covariant Neural Network for 4 Dimensional Non-Abelian Gauge Theory, http://arxiv.org/abs/2103.11965.

標題：Criticality and scale invariance in quantum Hall systems: plateau transitions and self-similarity of response functions

日時：2024 年 1 月 12 日(金) 午後 1 時 30 分～

場所：物性研究所本館 6 階 第 5 セミナー室 (A615)

講師：Gunnar Möller

所属：Physics and Astronomy, Division of Natural Sciences, University of Kent

要旨：

Since the realisation that quantum Hall liquids represent topologically ordered phases, the search for new topological states of matter has been a central endeavour in condensed matter physics. Interacting particles in flat band models provide a host of opportunities for creating novel topological phases, baptised fractional Chern insulators (FCI), which are based on realisations of synthetic magnetic fields. First materials realisations have recently been discovered in twisted $MoTe_2$ bilayers.

The interacting Hofstadter model gives blueprint examples for FCI phases, as predicted by composite fermion theory [1]. We will first review exact diagonalisation results for FCI states stabilised in single Chern bands, and demonstrate that finite-size effects are minimised in the quasi-continuum limit of perfectly flat bands near flux densities $n\varphi \rightarrow 1/|C|$ [2,3,4]. We will then discuss a new class of interaction-driven quantum Hall plateau transitions occurring in the Hofstadter model, which arise from the competition of Chern insulator states at weak interaction with FCI states realised at the same particle density for strong interactions. In one such case, our DMRG data at flux density $n\varphi$=3/11 presents a direct transition between a C=4 Chern Insulator and a ν =1/3 Laughlin state, and we examine its exotic critical properties [5]. Even in the non-interacting case, Chern insulators provide new phenomenology in quantum Hall plateau transitions. We will present data on the case of the Haldane model, where the topological C=1 Chern

insulator can be destabilised either by increasing disorder or by increasing the effective mass parameter. In our study of the critical behaviour of these two transitions [6], we demonstrate in particular that the mass-driven transition displays critical exponents which vary continuously with the disorder strength. Finally, going beyond ground state properties of quantum Hall systems, we will expose self-similar features of the dynamical response functions arising for a Laughlin state probed at energies lying above the scale of the single-particle gap [7].

Möller, G. & Cooper, N. R. Composite Fermion Theory for Bosonic Quantum Hall States on Lattices. Phys. Rev. Lett. 103, 105303 (2009).
Möller, G. & Cooper, N. R. Fractional Chern Insulators in Harper-Hofstadter Bands with Higher Chern Number. Phys. Rev. Lett. 115, 126401 (2015).
Andrews, B. & Möller, G. Stability of fractional Chern insulators in the effective continuum limit of Harper-Hofstadter bands with Chern number |C|>1. Phys. Rev. B 97, 035159 (2018).
Andrews, B., Neupert, T. & Möller, G. "Stability, phase transitions, and numerical breakdown of fractional Chern insulators in higher Chern bands of the Hofstadter model" Phys. Rev. B 104, 125107 (2021).
Schoonderwoerd, L., Pollmann, F. and Möller, G. Interaction-driven plateau transition between integer and fractional Chern Insulators, arxiv:1908.00988 – v2: 2022.
6 J. Mildner, M. D. Caio, G. Möller, N. R. Cooper, and M. J. Bhaseen, Topological Phase Transitions in the Disordered Haldane Model, arxiv:2312.XXXXX (in submission).
Andrews, B. & Möller, G. Self-similarity of spectral response functions for fractional quantum Hall states. Proc. R. Soc. A 479, 20230021 (2023).

標題：Electron spectro-microscopy of the local chemistry and structure of 2D materials
日時：2024 年 1 月 15 日(月) 午後４時～
場所：物性研究所本館 6 階 A615（第 5 セミナー室）& Online
講師：Dr. Jerzy T. Sadowski
所属：Center for Functional Nanomaterials, Brookhaven National Laboratory
要旨：

The ongoing miniaturization in technological devices and the progress in surface science demand novel instrumental methods for surface characterization on a length scale of only a few atomic distances. The combination of an x-ray photoelectron emission microscope (XPEEM) or low-energy electron microscope (LEEM) is a powerful technique for studying the dynamic and static properties of 2D materials surfaces and thin films including growth and decay, phase transitions, reactions, surface structure and morphology. It utilizes low energy electrons to image surfaces with few nm lateral resolution and atomic layer depth resolution. In the LEEM/XPEEM setup, when using the electron irradiation, the backscattered electrons, Auger and secondary electrons may be used, while photoelectrons, Auger and secondary electrons are utilized for imaging when sample is irradiated with photons. In this talk I will present examples of the application of the LEEM/XPEEM technique to the investigations of novel materials, including 2D layered materials, thin films, and adsorbate structures. I will also introduce the Center for Functional Nanomaterials (CFN) and National Synchrotron Light Source II (NSLS-II) user facilities at the Brookhaven National Laboratory for fabrication and characterization of 2D materials and beyond.

This research used resources of the Center for Functional Nanomaterials and the National Synchrotron Light Source II, which are U.S. Department of Energy (DOE) Office of Science facilities at Brookhaven National Laboratory, under Contract No. DE-SC0012704.

標題：強相関電子物質における多層膜試料の核磁気共鳴

日時：2024 年 1 月 19 日(金) 午前 11 時～午後 0 時

場所：Online

講師：山中 隆義 特任助教

所属：東北大学金属材料研究所

要旨：

近年の成膜技術の進歩によって、実に様々な物質が薄膜として作製可能になっている。この技術は物質の人工的な 2 次元化や表面・界面の効果の顕在化、電子状態を人工的に制御する技術としても注目されている。

このように膜試料は研究の舞台として重要であるが、その物質量が少ないためにミクロなプローブによる実験は困難である。核磁気共鳴法(NMR)もその例には漏れないが、強磁場を用いたりヘテロ構造を多層作製するなどの工夫で困難を幾らか克服可能となる。

本セミナーでは我々の成果である重い電子系人工超格子膜の研究を中心に[1, 2]，NMR による膜試料の研究例を紹介した。

[1] T. Yamanaka, et al., Phys. Rev. B 92, 241105 (2015).
[2] G. Nakamine, et al., Phys. Rev. B 99, 081115 (2019).

標題：Emerging Physics of Alternative Charge-Density Wave in 1T-Transition Metal Dichalcogenides

日時：2024 年 1 月 22 日(月) 午後 4 時～午後 5 時

場所：物性研究所本館 6 階 第 5 セミナー室 (A615)

講師：Gil-Young Cho

所属：Pohang University of Science and Technology (POSTECH)

要旨：

1T-transition metal dichalcogenides (TMD) have been an exciting platform for exploring the intertwinement of charge density waves and strong correlation phenomena. While the David star structure has been conventionally considered as the underlying charge order in the literature, recent scanning tunneling probe experiments on several monolayer 1T-TMD materials have motivated a new, alternative structure, namely the anion-centered David star structure. In this paper, we show that this novel anion-centered David star structure manifestly breaks inversion symmetry, resulting in flat bands with pronounced Rashba spin-orbit couplings. These distinctive features unlock novel possibilities and functionalities for 1T-TMDs, including the giant spin Hall effect, the emergence of Chern bands, and spin liquid that spontaneously breaks crystalline rotational symmetry. Our findings establish promising avenues for exploring emerging quantum phenomena of monolayer 1T-TMDs with this novel noncentrosymmetric structure.

標題：NanoTerasu **超高分解能軟 X 線 RIXS で挑む物性研究**

日時：2024 年 1 月 22 日(月) 午後 1 時～

場所：6 階第一会議室 & Online

講師：宮脇　淳

所属：量子科学技術研究開発機構　次世代放射光施設整備開発センター　主任研究員

要旨：

2024 年 4 月から運用が開始されるナノテラスでは、10 本のビームライン（共用 BL: 3 本、コアリション BL: 7 本）が建設・立ち上げ中で、超高分解能 共鳴非弾性軟 X 線散乱(RIXS)装置は共用 BL の 1 本として設置される。

RIXS は、物質に共鳴条件で X 線を照射し、散乱 X 線のエネルギーを計測して入射エネルギーとの差を求めることで、

低エネルギー励起のエネルギーと運度量の分散関係を得ることができる分光手法である。

固体には、電荷、軌道、スピン、格子の自由度があるが、RIXS はこれら全ての励起を観測することができ、物性研究には非常に適した手法である。ただし、目的の励起を観測するためには高いエネルギー分解能が必要であり、近年、Cu L-edge で 50 meV を切る装置が開発され、RIXS の真価を発揮しつつある[1,2]。

Nano Terasu の RIXS 装置では、分解能 10 meV という目標を掲げて、長らく設計、開発、建設を行ってきた[3]。

2024 年 1 月時点で、建設がおおむね完了し、4 月からの試験的共用を経て、2024 年度末の共用開始に向けて立ち上げ・調整を進めている。セミナーでは、ビームライン、RIXS 分光器の概要と建設状況について紹介し、利用研究に対する展望についても述べた。

[1] N. B. Brookes et al., Nucl. Instrum. Methods Phys. Res. A, 903, 175–192 (2018).
[2] K.-J. Zhou et al., J. Synchrotron Rad. 29, 563–580 (2022).
[3] J. Miyawaki et al., J. Phys. Conf. Ser. 2380, 012030 (2022).

標題：First-principles and machine learning study of anharmonic vibration and dielectric properties of materials
日時：2024 年 1 月 26 日(金) 午後 4 時～午後 5 時
場所：Online and Seminar Room 5 (A615), ISSP（Hybrid）
講師：Tomohito AMANO
所属：Department of Physics, The University of Tokyo
要旨：

The computational simulation of the dielectric response of materials is essential for both analyzing experimental spectra and developing new materials. To accurately calculate the dielectric function, the classical static charge is often insufficient, and the Born effective charges or the mass center of the Wannier function (Wannier center) are required to describe the dipole moments of a system.

For crystals, where the Born effective charges are used to calculate dipoles, we have combined the self-consistent phonon method [1] and the linear response theory to predict the dielectric function of highly anharmonic crystals. I will present the accuracy of our method through applications to strongly anharmoic rutile TiO2 [2].

For liquids, anharmonic phonon methods are not available, and one resorts to molecular dynamics (MD) simulations. To calculate the system dipoles efficiently and accurately, we have extended the previously proposed method predicting molecular dipoles [3] and developed a versatile machine-learning model of dipole moments predicting the Wannier centers assigned to the chemical bonds [4]. In this talk, I will present the applications to several liquid alcohols and discuss their dielectric properties.

[1] T. Tadano and S. Tsuneyuki, Phys. Rev. B 92, 054301 (2015).
[2] T. Amano, T. Yamazaki, R. Akashi, T. Tadano, and S. Tsuneyuki, Phys. Rev. B 107, 094305 (2023).
[3] A. Krishnamoorthy, K. Nomura, N. Baradwaj, K. Shimamura, et al, Phys. Rev. Lett. 126, 216403 (2021).
[4] T. Amano, T. Yamazaki, and S. Tsuneyuki, in preparation.

標題：物質科学におけるデータ同化手法開発と応用
日時：2024 年 1 月 29 日(月) 午後 4 時～午後 5 時
場所：物性研究所 6 階第 5 セミナー室（A615）及び Online（Hybrid）
講師：原嶋 庸介
所属：奈良先端科学技術大学院大学
要旨：

物質科学において本来理論と実験は共通の目標を持つものだが、専門性が細分化された結果、これらを協調させるためには橋渡しが必要である。データ同化はシミュレーションと実験データを統合することで予測モデルを構築する機械学習的技術であり、理論と実験の相乗効果が期待できる。本講演ではデータ同化による物性予測モデル構築の実例と、最近開発したデータ同化と Bayes 最適化を組み合わせた物質探索手法を紹介した。

標題：Towards the applications of ab initio Quantum Monte Carlo in Materials Science
日時：2024 年 1 月 29 日(月) 午後 1 時 30 分～午後 2 時 30 分
場所：物性研究所本館 6 階 第 5 セミナー室 (A615)
講師：中野 晃佑
所属：物質・材料研究機構 (NIMS), マテリアル基盤研究センター (CBRM)
要旨：

Ab initio quantum Monte Carlo (QMC) techniques [1], such as variational quantum Monte Carlo (VMC) and diffusion quantum Monte Carlo (DMC), are state-of-the-art numerical methods to obtain highly accurate many-body wave functions. These methods are essential when tackling challenging compounds that cannot be treated correctly within the Density Functional Theory (DFT) framework. In this seminar, I will talk about an overview of ab initio QMC methods and introduce our QMC packages, TurboRVB [2] and TurboGenius [3]. I will also talk about recent algorithmic progress in atomic force calculations using QMC. One of the major drawbacks that hinders widespread QMC applications, especially in the materials science community, is the lack of an affordable scheme to compute atomic forces consistent with the derivatives of the potential energy surface, a.k.a. unbiased atomic forces. This is trivial within the DFT framework, but it is one of the long-standing problems in QMC. Very recently, we have proposed a very efficient method to obtain unbiased atomic forces and pressures in the Variational Monte Carlo (VMC) framework, exploiting the gauge-invariant and locality properties of its geminal representation [4]. I will demonstrate the effectiveness of our method for Hydrogen and Chlorine molecules and for the cubic boron nitride crystal.

[1] W. Foulkes, L. Mitas, R. Needs, and G. Rajagopal, Rev. Mod. Phys. 73, 33 (2001).
[2] K. Nakano, et al. J. Chem. Phys. 152, 204121 (2020).
[3] K. Nakano, et al. J. Chem. Phys. 159, 224801 (2023).
[4] K. Nakano, et al. arXiv:2312.17608 (2023).

標題：Direct Visualization of Electronic Liquid Crystal Phases in Correlated Dirac Nodal Line Semimetal GdSbTe

日時：2024 年 2 月 2 日(金) 午後 2 時～

場所：物性研究所本館 6 階 第 5 セミナー室 (A615) & Online

講師：Prof. Tien-Ming Chuang

所属：Institute of Physics, Academia Sinica, Taipei, Taiwan

要旨：

Electronic liquid crystal (ELC) phases are spontaneous symmetry breaking states arisen from strong electron correlation in solids such as cuprates and iron pnictides. Topological materials with symmetry protected Dirac or Weyl fermions, however, are mostly weakly correlated so the occurrence of ELC is rare thereof. Here, we report a direct observation of ELC phases in Dirac nodal line (DNL) semimetal GdSbxTe2-x. We discover real-space electronic nanostructures of incommensurate checkerboard modulation and intense local nematic order. We show chemical substitution generates local electronic nematicity and increases Peierls instability towards incommensurate checkerboard modulation before undergoing a charge density wave – orthorhombic transition. We also observe nematicity in our quasiparticle scattering interference imaging, which detects linearly dispersive q-vectors, consistent with the calculated topological band structure scattering off C2-symmetric dopants. Our results on correlated DNL semimetal, GdSbxTe2-x highlight the importance of dopant atoms in the ELC phases, opening a pathway towards a further microscopic understanding of the interplay among disorder, topology and electron correlation.

標題：Hall-effect studies on unconventional quantum materials under challenging conditions

日時：2024 年 2 月 7 日(水) 午後 4 時～午後 5 時

場所：物性研究所 6 階第 5 セミナー室（A615）及び Online（Hybrid）

講師：Toni Helm

所属：Dresden High Magnetic Field Laboratory, Helmholtz Zentrum Dresden Rossendorf

要旨：

In order to uncover and understand the physics of topical quantum materials, experiments are pushed to their limits in terms of setup dimensions and resolution. Challenging conditions, such as very low temperatures, high pulsed-magnetic fields, strong pressures or microscopically small but well-defined sample dimensions are inevitable for successful investigations. We apply focused ion beam (FIB) micro-patterning for the fabrication of micron-scale structures from bulk single crystals suitable for high precision electrical transport experiments. This approach has proven a powerful tool for experiments on various compounds with intriguing transport properties. In particular, Hall effect signals can be optimized by means of reducing the sample thickness to few microns.

In this talk, I will exemplify some of our recent projects that benefited from FIB assisted patterning and uncovered new physics in topical materials [1-4]. In the first examples, I will show how we can contribute to the field of unconventional magnetism. I will present recent results from electrical-transport experiments that we combined with microscopic magneto-sensitive imaging tools. This enabled us to study finite size-effects and reveal the Hall signature, comprised of anomalous and topological contributions, of Antiskyrmions in the Heusler magnet Mn1.4PtSn [1] and that of Skyrmion bubbles in the hard magnet MnBi [2]. We, furthermore, study highly conductive heavy-fermion metals in pulsed magnetic fields up to 70 T. In our recent work on the potential spin-triplet superconductor UTe2, we revealed a correlation between the emergence of reentrant superconductivity in fields above 40 T and the vanishing of the anomalous Hall effect. The vanishing and reemerging of the Hall signature within a particular field-orientation range, hints at a field-induced compensation of magnetic exchange, the so-called Jaccarino-Peter effect, as the potential origin of reentrant high-field superconductivity in UTe2 [3,4].

[1] Winter, M., Goncalves, F.J.T., Soldatov, I., et al.
"Antiskyrmions and their electrical footprint in crystalline mesoscale structures of Mn1.4PtSn." Commun. Mater. 3, 102 (2022).
[2] He, Y., Schneider, S., Helm, T., et al.
"Topological Hall effect arising from the mesoscopic and microscopic non-coplanar magnetic structure in MnBi." Acta. Mater. 226, 117619 (2022).
[3] Niu, Q., Knebel, G., Braithwaite, D., Helm, T., et al.
"Evidence of Fermi surface reconstruction at the metamagnetic transition of the strongly correlated superconductor UTe2." Phys. Rev. Res. 2, 033179 (2020).
[4] Helm, T., Kimata, M., Sudo, K., et al.
"Field-induced compensation of magnetic exchange as the possible origin of reentrant superconductivity in UTe2." Nat Commun 15, 37 (2024).

標題：Spin Supersolidity and Giant Magnetocaloric Effect in a Triangular Lattice Quantum Antiferromagnet
日時：2024 年 2 月 14 日(水) 午前 10 時 30 分～午前 11 時 30 分
場所：Online
講師：Prof. Wei Li
所属：Institute of Theoretical Physics, Chinese Academy of Sciences
要旨：

Supersolid is an exotic quantum state of matter that emerges near absolute zero temperature. The spin supersolid spontaneously breaks both the lattice translational and spin rotational symmetries, forming a quantum magnetic analog of supersolid. Recently, using tensor network approaches [1,2], we determined the microscopic spin Hamiltonian of a Co-based quantum antiferromagnet Na2BaCo(PO4)2. We discovered that it represents a rare and nearly perfect realization of the easy-axis triangular lattice Heisenberg model, and therefore supports the long-sought spin supersolid state [4]. We further predict theoretically and, in conjunction with experimental collaborators, observe a significant entropic effect related to this unique and highly fluctuating spin state – spin supersolid cooling [5].

[1] B.-B. Chen, L. Chen, Z. Chen, WL, and A. Weichselbaum, Exponential thermal tensor network approach for quantum lattice models. Phys. Rev. X 8, 031082 (2018).
[2] Q. Li, Y. Gao, Y.-Y. He, Y. Qi, B.-B. Chen, and WL, Tangent Space Approach for Thermal Tensor Network Simulations of the 2D Hubbard Model. Phys. Rev. Lett. 130, 226502 (2023).
[3] Y. Gao, Y. Fan, H. Li, […], Y. Wan, and WL. Spin supersolidity in nearly ideal easy-axis triangular quantum antiferromagnet Na2BaCo(PO4)2. Npj Quantum Mater. 7, 89 (2022).
[4] J. Xiang, C. Zhang, Y. Gao, […], W. Jin, WL, P. Sun, G. Su, Giant magnetocaloric effect in spin supersolid candidate Na2BaCo(PO4)2, Nature 625, 270–275 (2024).

標題：Exploiting Hidden Low-Rank Structures in Physics
日時：2024 年 2 月 16 日(金) 午後 4 時～午後 5 時
場所：物性研究所本館 6 階 第 5 セミナー室 (A615)
講師：Hiroshi SHINAOKA
所属：Saitama University
要旨：

Tensor networks are a powerful tool for compressing wave functions and density matrices of quantum systems in physics.Recent developments have shown that tensor network techniques can efficiently compress many functions beyond these traditional objects.Notable examples include the solutions to turbulence in Navier–Stokes equations [1] and the computation of Feynman diagrams [2,3].These advancements have heralded a new era in the use of tensor networks for expediting the resolution of various complex equations in physics.

In this presentation, I will overview our recent research in this domain.Initially, I will discuss the compression of the space-time dependence of the correlation function in quantum systems [3] through the use of the "Quantics Tensor Train." [4,5] This method leverages the inherent length-scale separation in the system to efficiently represent the function.Our approach demonstrates solving diagrammatic equations in a compressed format.

Subsequently, I will introduce a novel and robust tool named "Quantics Tensor Cross Interpolation." [6] This method is designed to learn a quantics low-rank representation of a given function, showcasing the versatility and potential of tensor network techniques in handling complex functions in physics.

[1] N. Gourianov et al., Nat. Comput. Sci. 2, 30 (2022).
[2] Y. N. Fernandez et al., PRX 12, 041018 (2022).
[3] H. Shinaoka et al., PRX 13, 021015 (2023).
[4] I. V. Oseledets, Dokl. Math. 80, 653 (2009).
[5] B. N. Khoromskij, Constr. Approx. 34, 257 (2011).
[6] M. K. Ritter, …, H. Shinaoka and X. Waintal, PRL 132, 056501 (2024).

標題：座標変換不変な自由エネルギー地形の導出
日時：2024 年 2 月 21 日(水) 午後 4 時～午後 5 時
場所：物性研究所 本館 6 階第 5 セミナー室 (A615 号室) 及び Online（Hybrid）
講師：中村 壮伸
所属：産業技術総合研究所
要旨：

従来もちいられている自由エネルギー地形(FEL)の定義は、反応座標の選択に関して非物理的な依存性を示すため、普遍的な予測能力に欠けています[1]。ここでは、物理的に妥当な 3 つの要請に基づいて、与えられた反応座標に対する FEL の公式を一意的に導出します[2]。我々の FEL の公式は非物理的な座標依存性がなく、特殊な場合には従来の FEL の定義と一致します。さらに我々の FEL は、時系列データ解析によって得られる量、つまり確率分布と拡散行列だけで表現されます。これらの性質は、我々の FEL が普遍的な予測能力を持っていることを意味します。

[1] D. Frenkel, Eur. Phys. J. Plus 128, 10 (2013).
[2] T. N. https://arxiv.org/abs/1803.09034

標題： New magnetotransport phenomena in Fe-doped ferromagnetic semiconductors and quantum heterostructures

日時： 2024 年 2 月 21 日(水) 午後 1 時 15 分～午後 2 時 15 分

場所： 物性研究所本館 6 階 第 5 セミナー室 (A615)

講師： Dr. Le Duc Anh

所属： Department of Electrical Engineering and Information Systems, The University of Tokyo

要旨：

Ferromagnetic semiconductors (FMS), which inherit properties of both semiconductors and ferromagnetic materials, are realized by doping a certain amount (several %) of magnetic elements in semiconductors. In the past, most of the research has been dedicated to Mn-doped III-V FMSs, which are only P-type and the highest Curie temperature (T_C) is 200 K. Recently, we presented an alternative approach by using Fe instead of Mn as the magnetic dopants in narrow-gap III-V semiconductors like InAs, GaSb, and InSb. Using low-temperature molecular beam epitaxy (MBE), we have successfully grown both P-type FMS [(Ga,Fe)Sb] [1] and N-type FMSs [(In,Fe)As [2,3], (In,Fe)Sb [4]]. Intrinsic room-temperature ferromagnetism has been observed in $(Ga_{1-x},Fe_x)Sb$ with x > 23% [1] and $(In_{1-x},Fe_x)Sb$ with x > 16% [4].

In this talk, we present new novel magnetotransport physics in bilayer structures of a nonmagnetic (NM) material and an Fe-doped FMS, where a magnetic proximity effect (MPE) from the FMS is expected to affect the NM channel. The sample structure consists of InAs (thickness t = 15 – 40 nm)/(Ga,Fe)Sb (15 nm, 20% Fe) grown on AlSb buffer/semi-insulating GaAs (100) substrates (Fig. 1a,b). We found that a strong and long-range MPE is induced at the InAs/(Ga,Fe)Sb interface, resulting in a spontaneous spin splitting ΔE, as large as 18 meV, in the InAs channel[5,6]. Furthermore, this spin splitting ΔE can be largely modulated by applying a gate voltage V_g. We observed a giant even-parity magnetoresistance (~80% at 14 T), which we call proximity magnetoresistance (PMR) [5,6], and a large odd-parity linear magnetoresistance (OMR) [7], corresponding to a resistance change of 27% when the perpendicular-to-plane magnetic field B (=10 T) direction is reversed. The unprecedented large OMR was found to occur in the edge transport channels of the InAs thin film, due to simultaneous breaking of both the space inversion symmetry (SIS) and the time reversal symmetry (TRS) (Fig. 1a). These new features realized in the Fe-doped FMSs and their quantum heterostructures are particularly important for the applications of low-power and high-speed spin-based electronics. Furthermore, the gate-controllable spin splitting provides a mechanism to locally access Majorana fermions in InAs-based Josephson junctions [8]. These works were partly supported by Grants-in-Aid for Scientific Research, the CREST and PRESTO Programs of JST, the UTEC-UTokyo FSI program, Murata Science Foundation and Spin-RNJ.

標題： 研究戦略室セミナー：PRX What kind of papers we are looking for?

日時： 2024 年 2 月 22 日(木) 午後 4 時～午後 5 時

場所： 物性研究所本館 6 階 大講義室(A632)

講師： Dr. Yiming Xu

所属： Associate editor of Physical Review X

要旨： Speaker: Dr. Yiming Xu

(Associate Editor of Physical Review X)

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PRX's editorial and peer-review process effectively and get the most out of your interactions with the editors and referees? I will use the talk to discuss with you how to answer these questions. Many of these questions do not have a black-and-white answer in the case of a single paper. Open-minded, reasoned, and constructive dialogues amongst the authors, the editors, and the referees are key to making each concrete process a meaningful and productive experience, and sometimes even a pleasure, for everyone.

標題：Simulating endosomal escape of lipid nanoparticles: A coarse-grained molecular dynamics study
日時：2024 年 3 月 11 日(月) 午後 4 時～午後 5 時
場所：物性研究所 6 階第 5 セミナー室（A615）及び Oline（Hybrid）
講師：篠田　渉
所属：岡山大学 異分野基礎科学研究所
要旨：

We illustrate here our recent application study of our quantitative coarse-grained model; SPICA force field[1-4], to investigate the endosomal escape mechanism of lipid nanoparticles(LNPs). LNPs are one of the most promising non-viral gene delivery carriers.

LNPs have recently been employed in mRNA vaccines and are expected to have applications in cancer therapy and regenerative medicine. LNPs administered to the body enter the cell by endocytosis. Nucleic acids must be released into the cytoplasm before they are degraded by a drop in pH in the endosome (transfection), but in many cases, only a few percent are released.

The molecular mechanism is still elusive because it occurs at the nanoscale. Therefore, Clarifying this phenomenon through molecular dynamics (MD) simulations will enable a more effective design of LNPs with high drug release efficiency.

In this study, a series of large-scale coarse-grained MD simulations of LNPs fusing to endosomal membranes has been performed using the SPICA force field. In particular, the fusion mechanism of LNPs with the endosomal membrane was examined in the context of the efficiency of the endosomal escape.

We would also like to show the performance of the SPICA force field for this complex system, including a variety of lipids, sterols, and nucleic acids.

[1] Seo & Shinoda, J. Chem. Theory Comput. 15, 762 (2019).
[2] Kawamoto et al., J. Chem. Theory Comput. 18, 3204 (2022).
[3] Yamada et al., J. Chem. Theory Comput. 19, 8967 (2023).
[4] URL https://www.spica-ff.org/