物性研究所セミナー

標題：光化学反応の磁場効果
日時：2018 年 1 月 10 日(水)　午後 2 時～午後 3 時
場所：物性研究所本館 6 階 第 4 セミナー室（A614）
講師：谷本 能文
所属：広島大学
要旨：

化学・物理・生物に対する磁場効果の研究は、現在“磁気科学―Magneto-Science―”1 と呼ばれている。これらの磁場効果の主要なメカニズムは 4 つある。(1)ラジカル対機構、(2)異方的磁気エネルギー、(3)磁気力、(4)ローレンツ力である。(1)は光化学反応の磁場効果、(2)は結晶などの磁気配向、(3)は不均一反応の磁場効果や磁気浮上、(4)は不均一反応の磁場効果などの主なメカニズムである。ここでは、溶液中の有機光化学反応の磁場効果について概説する。

参考文献

M. Yamaguchi and Y. Tanimoto (eds.),Magneto-Science, Kodansha/Springer, Tokyo (2006).

R. De et al.,Chem. Phys. Lett., 315(1999) 381.

R. De et al., Bull. Chem. Soc. Jpn., 73(2000) 1573.

標題：Floquet topological phases protected by dynamical symmetry
日時：2018 年 1 月 10 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）
講師：Takahiro Morimoto
所属：UC Berkeley
要旨：

Nonequilibrium systems under periodic driving (Floquet systems) realize novel topological phases that cannot be achieved in equilibrium systems. One unique feature of periodically driven systems is that they can host a purely dynamical symmetry that involves time-translation. In this talk, we present a new class of Floquet topological phases protected by one realization of such dynamical symmetry, i.e., “time-glide symmetry” which is defined by a combination of reflection and time translation [1]. We introduce lattice models of free fermions with time-glide symmetric driving that show stable gapless surface states. We then give a general classification theory of time-glide symmetric Floquet topological phases by using a Clifford algebra approach. In addition, we also discuss Floquet topological phases of interacting bosons by showing examples in 1D and 2D systems [2,3].

[1] T.Morimoto, H.C. Po, and A. Vishwanath, Phys. Rev. B 95, 195155 (2017).

[2] A.C. Potter, T. Morimoto, A. Vishwanath, Phys. Rev. X 6, 041001 (2016).

[3] A. C. Potter and T. Morimoto, Phys. Rev. B 95, 155126 (2017).

標題：SARPES 2.0：obtaining information from spin interference
日時：2018 年 1 月 17 日(水)　午前 11 時～
場所：Seminar Room 5 (A615), 6th Floor,ISSP
講師：Prof. Hugo Dil
所属：Ecole Polytechnique Federale de Lausanne
要旨：

Over the last decades spin- and angle-resolved photoemission spectroscopy (SARPES) has developed into a powerful method to unravel the spin textures of a variety of materials. These spin textures are either determined by ferromagnetic properties or by spin-orbit interaction, as in the case of Rashba systems and topological materials. The insight obtained from such results is very rich, but mostly focusses on reconstructing the initial state spin properties. Based on changes in technical possibilities, recently a different way of looking at the spin in photoemission has encountered a revival, namely to consider the interference of spin channels. This can occur for spin-polarized or doubly degenerate initial states, but also lead to spin polarization in photoemission from spin-degenerate initial states.

In this talk I will give an introduction to SARPES and then focus on interference effects. It will be shown how this is related to the initial state properties, but also how it gives information about the photoemission process itself. For example, it allows us to determine the attosecond time-delay of photoemission. Recent results and the open questions that remain will be discussed together with future possibilities to further extend the obtained information.

標題：Electronic structure manipulation in polar and multiferroic materials
日時：2018 年 1 月 19 日(金)　午後 4 時～
場所：物性研究所本館 6 階 第 5 セミナー室 (A615)
講師：Hugo Dil
所属：Ecole Polytechnique Federale de Lausanne
要旨：

One of the main topics of moderns condensed matter physics is the design and verification of novel electronic structures. The toolbox available to alter the electronic properties is very large and ranges from the intrinsic crystal structure and symmetries to external fields. In this talk I will discuss how an intrinsic net electric dipole moment influences the electronic structure. Depending on the orientation of the dipole moment this can lead to a large (bulk) Rashba-type spin splitting or to the localisation of states. Both are easily detected by (spin- and) angle-resolved photoemission spectroscopy ((S)ARPES). A further functionality is added when this dipole moment can be manipulated or reversed, thus leading to ferroelectric order. It will be shown how the bulk spin texture of a ferroelectric semiconductor can be changed by applying an external electric field. In multiferroics the ferroelectric property is combined with ferromagnetic order, and in magnetoelectric materials the two order parameters are directly coupled. It will be shown how the spin texture is changed in such materials and how either magnetic or electric fields can be used to manipulate the electronic structure. The investigated systems include transition metal oxides and (magnetically doped) ferroelectric semiconductors.

標題：Topological aspects of nonlinear optical effects

日時：2018 年 1 月 23 日(火)　午前 10 時 30 分～11 時 30 分

場所：物性研究所本館 6 階 第 5 セミナー室（A615）

講師：Takahiro Morimoto

所属：UC Berkeley

要旨：

The responses of materials to high intensity light, i.e., nonlinear optical responses, constitute a vast field of physics and engineering. While topology has been playing a central role in recent studies of condensed matters, topological aspects of nonlinear optical effects have not been fully explored so far. In this talk, I will show a few examples of nonlinear optical effects that have topological origins. First, I discuss that the second-order nonlinear optical effects including the shift-current and second harmonic generation (SHG) are described by topological quantities, the Berry connection of Bloch wave functions [1]. Next, I show that the topological formula well explains giant SHG responses in Weyl semimetal that were observed in TaAs [2]. Finally, I discuss that another second-order nonlinear effect, circular photogalvanic effect (CPGE), is governed by Berry curvature and measuring CPGE in Weyl semimetals allows an access to monopole physics of Weyl fermions [3].

[1] T. Morimoto, and N. Nagaosa, Sci. Adv. 2, e1501524 (2016).
[2] Liang Wu, et. al., Nat. Phys. 13, 350 (2017).
[3] F. de Juan, A. G. Grushin, T. Morimoto, and J. E. Moore, Nat. Commun. 8, 15995 (2017).

標題：Multiscale modeling of the coarsening of connected structure and the thermal fluctuations of dislocations

日時：2018 年 1 月 26 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：Dr. Pierre-Antoine Geslin

所属：Institute for Materials Research, Tohoku University, Sendai Mateis lab, INSA/CNRS, UMR 5510, Lyon, France

要旨：

My talk will consist in two separate parts. The first part will focus on the coarsening of connected structures by surface diffusion. Nanoporous and microporous materials are of great interest in a number of applications ranging from battery anodes to captors and capacitors. When surface diffusion is thermally activated, these porous microstructures evolve in time, leading to a decrease of their surface area and a drop of the properties of the materials. Using a phase-field model for surface diffusion, we have investigated the coarsening behavior taking place during the evolution of these structures. More specifically, we have looked in details into the interactions between the morphological and topological characteristics of these structure during their evolution. The role of surface anisotropy on the coarsening kinetics have also been investigated.

The second part of my talk will focus on the thermal fluctuations of dislocations. The plastic behavior of metals and alloys are mostly controlled by the displacement of linear defects called dislocations. However, the behavior of these defects in temperature remains partially knows due to the complexity of the strain field generated in their vicinity. We have recently derived an analytical solution for the energy of a weakly perturbed dislocation., allowing us to characterize analytically the thermal fluctuations of dislocations. This analytical description matches remarkably well the fluctuation spectrum obtained from large scale molecular dynamics simulations, showing the validity of our

approach. This new model also opens the way to develop analytical treatment for various problems involving thermally activated dislocation movement (cross-slip, kink pair formation, obstacle bypassing,…)

標題：量子ビームイメージング技術のフロンティア開拓
日時：2018 年 2 月 1 日(木) 午後 2 時～
場所：物性研究所本館 6 階 第一会議室（A636）
講師：矢代 航
所属：東北大学多元物質科学研究所
要旨：

我が国は「ものづくりの国」とよくいわれるが、「ものづくり」と「計測」は、科学・技術の進歩における車の両輪である。すなわち、両者がバランスよく前進するべきであり、さもなくば迷走に陥るであろう。高度な職人技も、優れた五感があればこそ、であり、人間の感覚を遙かに超えた最先端のものづくりにおいても、計測技術のフロンティアの開拓が不可欠である。

本講演では、特に量子ビーム（主にX線および中性子）イメージング技術のフロンティア開拓に焦点を絞り、私が近年取り組んできた研究の成果などについて紹介する。一般に計測法のフロンティアの開拓は、自然現象の基本的な理解にはじまり、計測法の確立に向けた計測系、計測素子・機器、シミュレーション・解析法の研究・開発、さらには製品化に向けた汎用機器の開発という展開によって、はじめて本質的な意味で進展するものである。本講演では、このような本質的な進展を目指して講演者が取り組んできた、量子ビームイメージング技術のフロンティア開拓に向けた分野横断的な研究について紹介する。

X線、中性子イメージング法のフロンティアの開拓は、具体的には、高密度分解能化、高空間分解能化、高時間分解能化、大視野化、多次元化などに代表される。これらのフロンティアの開拓には、X線・中性子光学の理論・実験両面の基礎研究だけでなく、従来の限界を超える高度な微細加工技術の開拓、高度な情報処理技術の開拓など、分野横断的な研究が不可欠である。本講演ではそのような新たな展開の例として、新規材料による高アスペクト比X線光学素子の開発[1]や、高度情報処理技術との融合によるミリ秒トモグラフィ法の開発[2]（JST CREST（2017 年 10 月開始））、さらには、多次元化に向けた新たな挑戦として、表面・界面構造解析とイメージング技術の融合に向けた取り組み[3]や、医療診断へ向けたX線エラストグラフィ法の開発（AMED 先端計測分析技術・機器開発プログラム（2017 年 8 月開始））などについても紹介する。

[1] W. Yashiro et al., Appl. Phys. Express 7 (2014) 032501; W. Yashiro et al., Jpn. J. Appl. Phys. 55 (2016) 048003.
[2] W. Yashiro et al., Appl. Phys. Express 10 (2017) 052501; Jpn. J. Appl. Phys. 56 (2017) 112503.
[3] W. Yashiro et al., Opt. Express 18 (2010) 16890-16901; W. Yashiro et al., Phys. Rev. B 84 (2011) 094106; W. Yashiro et al., Opt. Express 23 (2015) 9233-9251; W. Yashiro et al., Jpn. J. Appl. Phys. 53 (2014) 05FH04.

標題：STM studies of FeSe single crystals
日時：2018 年 2 月 8 日(木)　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：Prof. Maria Iavarone
所属：Department of Physics, Temple University, USA
要旨：

In spite of its simple crystal structure, the electronic properties of the iron-based superconductor FeSe (Tc ~ 9 K) are rich and attractive. Superconductivity in FeSe takes place in a so-called nematic phase that is associated with orbital ordering. Another interesting aspect is that Fermi wave length is as long as the coherence length therefore, placing FeSe most likely in the BCS-BEC crossover regime. These features should result in non-trivial electronic states around the local defects such as vortices and impurities. We have performed low temperature STM/STS experiments on FeSe to investigate its electronic structures. Multiband superconductivity aspects, symmetry of the order parameter, role of disorder, vortex matter and chemical substitution effects on the band structure of this system will be discussed.

標題：遷移金属二硫化物 WS2 を用いたグラフェンへの異方的スピン軌道相互作用の誘起
日時：2018 年 2 月 13 日(火)　午後 2 時～午後 3 時
場所：物性研究所本館 6 階 第 5 セミナー室（A615）
講師：若村 太郎
所属：パリ南大学
要旨：

内因的なスピン軌道相互作用が極めて小さいグラフェンへの強いスピン軌道相互作用の誘起は、スピントロニクスへの応用や、量子スピンホール状態など新奇な物性の発現への期待から、近年盛んに研究が行われている。その中でも特に、グラフェンと同様の 2 次元層状物質であり、強いスピン軌道相互作用を持つ遷移金属二硫化物とグラフェンの積層構造を作製し、界面での相互作用を通してグラフェンのスピン軌道相互作用を増大させる手法が注目を集めている。

本研究では、グラフェンと遷移金属二硫化物 WS2 の積層構造を作製し、グラフェンに誘起されるスピン軌道相互作用の大きさを弱反局在効果の測定により評価した。遷移金属二硫化物は膜厚によってバンド構造などの特性が変化するため、WS2 として単層、およびバルクの 2 種類を用いて素子を作製し、比較を行った。低温での磁気抵抗効果の測定の結果、WS2 が単層の場合とバルクの場合の両方で強いスピン軌道相互作用が誘起されたことを示す弱反局在効果が観測され、特に WS2 が単層の場合、バルク WS2 の場合と比較して 1 桁以上大きいスピン軌道相互作用を見積もることが出来た。さらに誘起されたスピン軌道相互作用の対称性についても詳しく考察を行ったところ、弱反局在効果の解析から、グラフェン–単層 WS2/バルク WS2 両方の系において対称的なスピン軌道相互作用が支配的であることが分かった。

これらの結果は、グラフェン–単層 WS2 構造がグラフェンにより効率的に強い面対称的スピン軌道相互作用を誘起可能であり、グラフェンでの量子スピンホール状態の実現に有用な系であることを示唆している。本発表では、上記の内容に加えてグラフェン–単層 WS2 構造で見られた異常な抵抗の温度依存性、スピン緩和機構とスピン軌道相互作用の対称性の関連について、またヴァレー–ゼーマン型スピン軌道相互作用の存在についても議論する予定である[1]。

[1] T. Wakamura et al., arXiv :1710.07483 (2017).

標題：Symmetric tensor networks and topological phases
日時：2018 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：Ying Ran
所属：Boston College and ISSP
要旨：

I will describe a theoretical framework to systematically classify and construct generic tensor-network wavefunctions (in d=1,2,3 spatial dimensions) respecting both onsite and spatial symmetries, which turns out to be directly related to topological phases and useful from both conceptual and practical points of view. For example, on the conceptual side, this framework allows us to (partially) classify general symmetry protected topological phases involving spatial symmetries, and to prove a generalized Lieb-Schultz-Mattis theorem involving general magnetic translations. We also identify a generic connection between SPT phases and rather conventional symmetry enriched topological (SET) phases via an anyon condensation mechanism, which may serve as a guideline to search for SPT phases in realistic models. On the practical side, the constructed generic tensor-network wavefunctions are useful for variational numerical simulations.

[References: arXiv:1505.03171, 1509.04358, 1610.02024, 1611.07652, 1705.05421]

標題：Cavity QED in the Ultrastrong Coupling Regime
日時：2018 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 第一会議室（A636）
講師：河野 淳一郎
所属：Departments of Electrical and Computer Engineering, Physics and Astronomy, and Materials Science and NanoEngineering, Rice University, Houston, Texas, U. S. A
要旨：

Strong resonant light-matter coupling in a cavity setting is an essential ingredient in fundamental cavity quantum electrodynamics (QED) studies as well as in cavity-QED-based quantum information processing. In particular, a variety of solid-state cavity QED systems have recently been examined, not only for the purpose of developing scalable quantum technologies, but also for exploring novel many-body effects inherent to condensed matter. This talk will first describe our recent observation of collective ultrastrong light-matter coupling in a 2D electron gas in a high-quality-factor terahertz cavity in a quantizing magnetic field, demonstrating a record-high cooperativity [1]. The electron cyclotron resonance peak exhibited splitting into the lower and upper polariton branches with a magnitude that is proportional to the square-root of the electron density, a hallmark of collective vacuum Rabi splitting. The second part of this talk will present 1D microcavity-exciton-polaritons in a thin film of aligned carbon nanotubes [2] embedded in a Fabry-Perot cavity, also exhibiting collective ultrastrong light-matter coupling. These experiments open up a variety of new possibilities to combine the traditional disciplines of many-body condensed matter physics and cavity-based quantum optics.

References

1. Q. Zhang et al., Nature Physics 12, 1005 (2016).
2. X. He et al., Nature Nanotechnology 11, 633 (2016).

標題：A Monte-Carlo study of three-dimensional chiral spin liquids in anisotropic hypernonagon Kitaev models

日時：2018 年 2 月 21 日(水)　午後 3 時～午後 4 時

場所：物性研究所本館 6 階 第 5 セミナー室（A615）

講師：加藤 康之

所属：Department of Applied Physics, University of Tokyo

要旨：

The Kitaev model is an exactly-soluble quantum spin model with frustration. Since the ground state was rigorously proven to be a quantum spin liquid, this model has been extensively studied in this decade. Although the original model was defined on a simple honeycomb lattice, the model has been extended to various tricoordinate lattices without losing the exact solubility. We analyze two different anisotropic limits of the Kitaev model on a three-dimensional lattice comprising nine-site elementary loops, which we call the hypernonagon lattice. In both cases, the effective Ising-type models retain the time-reversal symmetry, suggesting that the ground states are chiral spin liquids. Using Monte Carlo simulations that respect the local and global constraints on the Ising variables representing Z2 fluxes, we show that there is a first-order phase transition at a finite temperature in each case, but in a different manner.

Reference: Y. Kato, Y. Kamiya, J. Nasu, and Y. Motome, Phys. Rev. B 96, 174409 (2017).

標題：Symmetry enhanced first-order phase transition in a two-dimensional quantum antiferromagnet

日時：2018 年 2 月 21 日(水)　午前 10 時～午前 11 時

場所：物性研究所本館 6 階 第 5 セミナー室（A615）

講師：Prof. Anders W. Sandvik

所属：Boston University and Institute of Physics, Chinese Academy of Sciences

要旨：

Theoretical descriptions of quantum phase transitions have indicated the existence of critical points with higher symmetry than those of the underlying Hamiltonian. Points of emergent symmetry have not been expected at discontinuous (first-order) transitions, however. I will discuss such an example [1], where phase coexistence at a first-order transition takes the form of an enhanced rotational symmetry in a space of two order parameters. Using quantum Monte Carlo simulations to study a 2D S=1/2 quantum magnet hosting the antiferromagnetic (AFM) and plaquette singlet (PS) states recently detected in SrCu2(BO3)2, we observe that the O(3) symmetric AFM order and the Z2 symmetric PS order form an O(4) vector at the transition. The control parameter (a coupling ratio) rotates the vector from the AFM sector to the PS sector, with the length of the combined order parameter vector always remaining non-zero. This phenomenon should be observable in neutron scattering experiments on SrCu2(BO3)2.

[1] B. Zhao, P. Weinberg, A. W. Sandvik (in preparation)

標題：Photoinduced reaction dynamics of nanocarbons
日時：2018 年 2 月 21 日(水)　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：山崎 馨
所属：Institute for Materials Research, Tohoku University, Sendai, Japan
要旨：

Nanocarbons such as fullerene, carbon nanotube, and graphene are the fundamental materials for carbon-based nanotechnologies. Their optical and electronic properties heavily depend on their size and shape. In order to realize single-molecule scale structural engineering of nanocarbons using laser irradiation, we quantum-chemically investigated the mechanism of the photoinduced reaction dynamics of nanocarbons both in energy and time domains.

We first investigated the reaction paths of Stone–Wales rearrangement (SWR), i.e., π/2 rotation of two carbon atoms with respect to the midpoint of the bond, in graphene and carbon nanotube at the MS-CASPT2//SA-CASSCF level of multi-reference molecular orbital theory [1]. We found that the vibronic (electron-phonon) coupling play a crucial role to reduce the effective reaction barriers of the photoinduced defect formation of nanographene.

We next investigated that the fragmentation dynamics of the highly charged fullerene cation $C60q+$ (q = 20-60) produced by the irradiation of x-ray free electron laser pulse using on-the-fly classical trajectory calculations combined with density functional based tight-binding theory. We found that a two-step explosion mechanism governs the fragmentation dynamics [2]: $C60q+$ firstly ejects singly and multiply charged fast atomic cations $Cz+$ ($z \geq 1$) to reduce its strong intramolecular Coulomb repulsion on a timescale of 10 fs. Thermal (statistical) evaporations of slow atomic and molecular fragments from the remaining core cluster subsequently occur on a timescale of 100 fs to 1 ps.

I will also briefly discuss our recent results on the real-time imaging of the near-/mid-IR induced coherent vibration of C60, which is considered as the initial step of the photoinduced fragmentation of C60 [3]

References:

[1] K. Yamazaki et al., J. Phys. Chem. A 116, 11441 (2012).
[2] K. Yamazaki et al., J. Chem. Phys. 141, 121105 (2014).
[3] K. Yamazaki et al., to be submitted.

標題：Exchange interaction in magnetic topological insulators and related materials
日時：2018 年 2 月 23 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：Prof. Arthur Ernst
所属：Johannes Kepler Universität Linz, Max-Planck-Institut für Mikrostrukturphysik
要旨：

It is a well known fact that a magnetic field can break the time reversal symmetry and therewith can destroy a topologically protected surface state in topological insulators. However, the interplay between magnetism and topological order can yield a number of interesting phenomena such as the quantum anomalous Hall effect, a topological magneto-electric effect, and quantized Kerr- or Faraday rotation. This motivates researcher for a search of new magnetic topological insulators and for an intensive study of their electronic and magnetic properties. In my talk, I'll give an overview of our first-principles investigations on this class of materials. In the first part, I'll present a method and approximations used in our simulations and then talk about several examples of magnetic topological insulators, studied in our group within the last three years. First of all, I'll discuss topological insulators doped with magnetic impurities, which can imply various magnetic order in these materials. A special attention will be devoted to

the exchange interaction between magnetic impurities and to the impact of electron-magnon interaction on the electronic structure in some doped topological systems. As next, I'll demonstrate how some defects or impurities without magnetic moments can induce magnetism in topological insulators and discuss the main features of magnetic interactions in these systems.

標題：Weyl magnons in pyrochlore antiferromagnets with all-in- all-out orders
日時：2018 年 3 月 14 日(水)　午前 10 時 30 分～午前 11 時 30 分
場所：物性研究所本館 6 階 第 5 セミナー室 (A615)
講師：Dr. Wenxing Nie
所属：Sichuan University, China
要旨：

In this talk, I will introduce our recent work about the investigation of novel topological magnon band crossings in pyrochlore antiferromagnets with all-in- all-out (AIAO) magnetic order. I will show that by the combination of general symmetry analysis and spin-wave theory, we find that pyrochlore materials with AIAO orders can host Weyl magnons under external magnetic fields or uniaxial strains. Under a small magnetic field, the magnon bands of the pyrochlore with AIAO background can feature two opposite-charged Weyl points, which is the minimal number of Weyl points realizable in quantum materials and has not be experimentally observed so far.
We further show that breathing pyrochlores with AIAO orders can exhibit Weyl magnons upon uniaxial strains. These findings apply to any pyrochlore material supporting AIAO orders, irrespective of the forms of interactions. Specifically, we show that the Weyl magnons are robust against direct (positive) Dzyaloshinskii-Moriya interactions. Because of the ubiquitous AIAO orders in pyrochlore magnets including R2Ir2O7, and experimentally achievable external strain and magnetic field, our predictions provide promising arena to witness the Weyl magnons in quantum magnets.

Ref: S-K. Jian and W.-X. Nie, arXiv: 1708.02948

標題：Insensitivity of bulk properties to the twisted boundary condition
日時：2018 年 3 月 16 日(金)　午後 1 時 15 分～午後 2 時:45 分
場所：Seminar Room A at Kavli IPMU
講師：Haruki Watanabe
所属：Dept. Applied Physics, University of Tokyo
要旨：

The symmetry and the locality are the two major ingredients leading to various nontrivial statements in quantum many-body systems. In this talk I will show that, in gapped phases of a U(1) symmetric Hamiltonian with finite-range interactions, the bulk properties such as the expectation value of local operators, the ground state energy and the excitation gap, and the static and low-frequency dynamical responses in general, do not depend on the twisted angle of the boundary condition in the limit of the large system size. The argument is based on the exponential decay of several types of equal-time correlation functions.

Remark: joint with IPMU Mathematics-String Theory seminar