物性研究所セミナー

標題：理論セミナー：Earth & Planetary Materials (to be) Explored by K and Fugaku Supercomputers and Quantum Beamlines

日時：2019 年 12 月 20 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：飯高 敏晃

所属：理化学研究所

要旨：

Behavior of materials in deep Earth and planets, such as silicate minerals, iron alloys, water and hydrogen- and helium- gases in solid and liquid states, are still almost unknown. Our goal [1] is to establish the basic knowledge of these materials to understand the history of Earth and planets by combining the first principles quantum calculations on K and Fugaku Supercomputers with diffraction and spectroscopy measurements at quantum beamlines such as SPring-8, SACLA, and J-PARC.

In this talk I will introduce our calculation of X-ray Raman scattering spectrum of solid oxygen [2,3].

[1] Post-K Exploratory Challenge 1-1-C, "Structure and Properties of Materials in Deep Earth and Planets".
http://www.iitaka.org/~xmat/

[2] H. Fukui et al., PNAS, 201905771 (2019).
http://dx.doi.org/10.1073/pnas.1905771116

[3] L. T. Anh et al., Sci. Rep. 9, 8731 (2019).
http://dx.doi.org/10.1038/s41598-019-45314-9

標題：LASOR **セミナー：**Topological kagome magnet -Mn3Sn and Fe3Sn2

日時：2019 年 12 月 23 日(月)　午前 11 時～午後 0 時

場所：物性研究所本館 6 階 第 5 セミナー室(A615)

講師：朱宮 奈那

所属：プリンストン大学

要旨：

Owing to the unusual geometry of kagome lattices, their electrons are useful for studying the physics of frustrated, correlated and topological quantum electronic states. In the presence of strong spin–orbit coupling, the magnetic and electronic structures of kagome lattices are further entangled, which can lead to hitherto unknown spin–orbit phenomena. In this talk, I will discuss two of the kagome magnets we studied, Mn3Sn and Fe3Sn2, using a scanning tunneling microscopy with a vector-magnetic- field capability and temperature control.

Mn3Sn is a strongly correlated antiferromagnet consisting of only kagome layers. We observe a pronounced resonance with a Fano line shape at the Fermi level resembling the Kondo resonance previously observed in some f-electron materials. The magnetic field and temperature dependence indicate its strongly interacting nature. Our new results uncover the emergent many-body resonance behavior in an antiferromagnetic topological material but without f-electrons.

Fe3Sn2 is a ferromagnet containing a kagome bilayer. We discover that its many-body electronic state couples strongly to the vector field with three-dimensional anisotropy, exhibiting a giant nematic energy shift. We further manipulate the nematicity with our vector magnetic field due to its giant spin-driven electronic responses, which points to the realization of an underlying correlated magnetic topological phrase. It provides new ways of controlling spin-orbit properties and exploring emergent phenomena in topological quantum materials [1].

[1] Yin, J., Zhang, S.S. et al. Nature 562, 91–95 (2018).

標題：ナノサイエンスセミナー：Nanoscopy of charge fluctuations in matter – Scanning Noise Microscope (SNoiM)-

日時：2019 年 12 月 26 日(木)　午後３時～午後４時

場所：物性研究所本館６階 第３セミナー室(A613)

講師：Dr. Qianchun Weng (**翁 銭春**)

所属：Surface and Interface Science Laboratory, RIKEN

要旨：

All material generates fluctuating electromagnetic (EM) evanescent field on its surface due to charge/current fluctuations, which are thermally agitated (thermal noise) or non-thermally excited (excess noise or shot noise). In general, current fluctuation (or noise) in a nanoscale region of the material carries key information of the local thermal/nonequilibrium phenomenon taking place at the given point [1]. In this seminar, I will describe an unprecedented novel microscope, called terahertz (THz) scanning noise microscope (Fig. 1(a)), which maps ultrahigh frequency (15-30 THz, 1 THz= 1012 Hz) current fluctuation with nanoscale spatial resolution. THz SNoiM is demonstrated to be a powerful and unique experimental tool for studying local nonequilibrium dynamics in a variety of material systems [2-4]. The example shown in Fig. 1(b) is the first direct visualization of hot electrons in a GaAs/AlGaAs quantum well (QW) device, which reveals the fundamental nature of non-local hot electron energy dissipation [4]. Physical processes probed by SNoiM are inaccessible with any other currently known methods. Particularly, it has been demonstrated [5] that conventional near-field microscope with external light excitation is unable to image the same phenomena that are visualized by SNoiM.

Reference:

[1] S. Komiyama, J. Appl. Phys. 125, 010901 (2019).
[2] S. Komiyama et al., arXiv: 1601.00368.
[3] Q. Weng et al., Nano Lett. 18, 4220 (2018).
[4] Q. Weng et al., Science 360, 775 (2018).
[5] Q. Weng et al., Appl. Phys. Lett. 114, 153101 (2019).

標題：理論セミナー：第一原理計算を用いた磁性体物性予測

日時：2019 年 12 月 27 日(金)　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：是常 隆

所属：東北大学理学研究科物理学専攻

要旨：

近年、ワイル点やベリー曲率といったバンドのトポロジカルな性質に着目した研究が盛んに行われている。強磁性体においては、これらは異常ホール効果や異常ネルンスト効果といった物理量につながることが知られている。このバンドのトポロジカルな性質は、第一原理的に得られたバンド構造を有効模型（タイトバインディング模型）で表すことによって、効率的に計算することが可能となる。

本セミナーでは、まずこのバンドのトポロジカルな性質と物性の関係[1]について概観し、強磁性体や Mn3Sn などにおける異常ホール効果や異常ネルンスト効果などの計算例を紹介する[2]。次に、この有効模型を作成する際に用いられる wannier90 と呼ばれるコードの最新版[3]について紹介し、これを用いた有効模型自動作成手法について説明する。この自動化手法を結晶構造データベースに適用して得られた強磁性体数千個に対する有効模型のリスト、およびそれを用いて得られた異常ホール効果、異常ネルンスト効果のデータベースについても紹介する。また、これらの物性値が結晶構造などの情報からどれほど予想できるのかを、機械学習を用いて解析した結果についても紹介する[4]。

[1] N. Nagaosa et al. Rev. Mod. Phys. 82 1539 (2010).

[2] M.-T. Suzuki et al. Phys. Rev. B 95 094406 (2017).

[3] G. Pizzi et al. Journal of Physics: Condensed Matter (2019). (arxiv:1907.09788).

[4] T. Koretsune et al. in preparation.

標題：ナノサイエンスセミナー：Programming electronic and spin states in 2D supramolecular architectures by modifications on the single atomic or molecular level

日時：2020 年 1 月 10 日(金)　午前 10 時 30 分～午前 11 時 30 分

場所：物性研究所本館６階　第２会議室(A635)

講師：Thomas A. Jung

所属：Paul Scherrer Institute and University of Basel, Switzerland

要旨：

Future quantum technologies rely on the understanding of the interaction between different electronic states in atoms or molecules. Surface supported atomic and molecular systems provide a base for such investigations with the particular advantage of addressability. In our work we establish on-surface architectures which exhibit extraordinary magnetic and quantum properties originating from the reduced dimensionality of the self-assembled and atomically precise architectures.

Quantum well arrays, exhibiting band-like electronic states [1] for example, can be produced by the interaction of porous on-surface networks with 2D Shockley-type surface states. These quantum wells have been modified by the adsorption / condensation of Xe atoms [2,3]. By designing the Xe filling pattern in the array, a quantum breadboard can be realized in remembrance of the breadboards used for testing electronic circuitry.

2D ‘checkerboard’ architectures of magnetic molecules containing different e.g. Fe, Mn spins, on exhibit particular magnetic properties and serve as templates for the modification of spins by e.g. ligands. On magnetic substrates their spin state is strongly determined by the substrate and can be selectively switched by ligation to e.g. NH3 [4]. On nonmagnetic Au(111), we have observed the first example of 2D ferrimagnetic long-range order and remanence due to the RKKY interaction mediated by the surface states of the support [5].

Self-assembled 2D architectures contribute to our understanding of fundamental interactions involved in low dimensional systems. In addition, we can put these in the framework of existing models towards their further development.

Reference
[1] Lobo-Checa, J. et al., Science 325, 300, (2009)
[2] Nowakowska, S. et al., Nat. Commun.
DOI: 10.1038/ncomms7071, (2015)
[3] Nowakowska, S. et al., Small 12, 3757, (2016)
[4] Ballav N., et al., JPCL, 4, 2303, (2013)
[5] Girovsky, J. et al., Nat. Commun.
DOI: 10.1038/ncomms15388, (2017)

標題：理論セミナー：Exploration on Deconfined Fractionalized Particles at Quantum Criticality: Fractional Chern Insulators and Quantum Magnets
日時：2020 年 1 月 14 日(火)　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：Jong Yeon Lee
所属：Harvard University
要旨：

One of the most exotic phenomena in condensed matter systems is the emergence of fractionalized particles. However, until now, only a few experimental systems are known to realize fractionalized excitations. This calls for more systematic ways to find and understand systems with fractionalization. One natural starting point is to look for an exotic quantum criticality, where the fundamental degrees of freedom become insufficient to describe the system accurately. Furthermore, understandings in exotic quantum critical phenomena would provide a unified perspective on nearby gapped phases, i.e. a guiding principle to engineer the system in a desirable direction that may host anyons. In this talk, I would present my works on quantum phase transitions between fractional Chern/Quantum Hall insulators tuned by the strength of lattice potential [PRX 8, 031015 (2018)]. Here, the low-lying excitations are already fractionalized; therefore, the deconfined fractional excitations follows more naturally, which is described by Chern-Simons quantum electrodynamics. The numerical results using iDMRG as well as theoretical analysis of their emergent critical properties would be presented. In the end, I would discuss their spectroscopic signatures, providing a full analysis of experimental verification. If time allows, I would talk about my other recent works on quantum magnets in 1+1 dimension.

標題：ナノサイエンスセミナー：Chiral recognition, spin filtering and molecular machines in two-dimensional molecular systems

日時：2020 年 1 月 17 日(金)　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：Karl-Heinz Ernst

所属：Empa, Swiss Federal Laboratories for Materials Science and Technology and University of Zurich, Switzerland

要旨：

Molecular recognition among chiral molecules on surfaces is of paramount importance in biomineralization, enantioselective heterogeneous catalysis, and for the separation of chiral molecules into their two mirror-image isomers (enantiomers) via crystallization or chromatography. Understanding the principles of molecular recognition in general, however, is a difficult task and calls for investigation of appropriate model systems. One popular approach is thereby studying intermolecular interactions on well-defined solid surfaces, which allows in particular the use of scanning tunneling microscopy (STM). Examples of chiral amplification via the so-called 'sergeant-and-soldiers' effect as well as manipulation of chiral adsorbates via inelastic electron tunneling will be presented. In a Pasteur-type experiment at the nanoscale, molecules that constitute a dimer are spatially separated with a molecular STM tip and their absolute handedness is determined with submolecular resolution STM.

Moreover, we report spin-dependent filtering of electrons by monolayers of these helical molecules. Finally, the first successful electrical current-driven unidirectional motion of a synthetic molecule, the so-called nanocar, will be presented and compared to recent results obtained for smaller molecular machines propelled by inelastic electron tunneling.

標題：理論セミナー：Ab initio molecular properties on a quantum computer: Green's functions and response functions

日時：2020 年 2 月 14 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：Taichi KOSUGI

所属：Tokyo Institute of Technology

要旨：

Since the information carrier of a programmable quantum computer is a set of qubits that exploits the principle of superposition, essentially parallel algorithms can exist and perform computation for classically formidable problems. Quantum chemistry is believed to be one of the most suitable research fields for quantum computation since its problem setting is quantum mechanical by definition. There exist multiple ab initio approaches to obtain the ground state of an interacting electronic system such as the variational quantum eigensolver (VQE) [1] and imaginary-time evolution [2]. Apart from which approach is adopted among them, the need for calculation of various physical properties of the target system arises. We proposed recently schemes for the construction of Green's function [3] and linear-response functions [4] of an interacting electronic system by using statistical sampling on a quantum computer. We performed classical simulations of such construction for molecular systems by comparing with the accurate ones based on the full configuration interaction calculations. The details of schemes and the results of simulations will be explained in the talk.

[1] Peruzzo et al., Nat. Commun. 5, 4213 (2014).
[2] Jones et al., Phys. Rev. A 99, 062304 (2019).
[3] Kosugi and Matsushita, Phys. Rev. A 101, 012330 (2020).
[4] Kosugi and Matsushita, arXiv:1911.00293

標題：セミナー：材料研究所の集客がなぜ４年で９倍増したのか ～若者が人生を変える科学広報とは～
日時：2020 年 2 月 20 日(木) 午前 10 時 30 分～午前 11 時 30 分
場所：物性研究所本館 6 階 大講義室(A632)
講師：小林 隆司
所属：物質・材料研究機構
要旨：

YouTube 登録者 10 万人超え。イベント 6 年連続集客記録更新…。

ＮＩＭＳは、地味で難解なはずの材料研究の世界に多くの若者を引き込み続けています。宇宙で大人気のＪＡＸＡをも超える高い訴求力を発揮しているため、Google から表彰され、Yahoo！から提携を希望されるなど注目を集めています。

専門家以外の人に科学を伝えるとき、重要なのは「論理的」であることでしょうか。 本当はそれ以上に大切なのに、ほとんどの科学者が無視していることがあります。反対に、テレビ番組をつい最後まで見てしまう理由はなんでしょうか。答えは「逆算」ができているかどうかです。

考えたこともなかった、伝える技術。テレビが使うあの手とこの手、その一部をお伝えします。

「ＮＩＭＳのおかげで中学時代に興味を持ち材料系の大学に進学を果たした」「教科書を作って欲しい」「ＮＩＭＳで研究をしたい」などの投稿が、次世代を担う若者から続々と寄せられてくる秘密はいったいどこにあるのでしょうか。
ヒントは、難しい数式を避けるのではなく、その難解な数式を知りたくて仕方なくなるような『気持ちを作る』こと。

若者を惹きつけてやまないＮＩＭＳ広報が実践する「科学の伝え方」。この１時間で、あなたの持つ「コミュニケーション」の意味がガラリと変わるのではないでしょうか。本にも教科書にもない『伝える技術』。体感していただきましょう。