物性研究所セミナー

標題：理論セミナー：Self-organization of Golgi body during mammalian cell division
日時：2017 年 1 月 16 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：立川 正志
所属：理化学研究所
要旨：

Our (eukaryotic) cells have a complex structure consisting of various organelle; cellular subunits made of lipid membrane. Organelle allows cells to carry various chemical reactions in parallel, to realize complex cellular functions and to construct complex multicellular organisms. However, because of the small size, the organization mechanism of the cellular complex structure remains elusive. In this study, we consider organization of Golgi body; a membrane-bound organelle working as the hub of the cellular logistics. Golgi body has a characteristic morphology; several flattened of lipid membrane sacs (cisternae) stacking to each other. At the cell division in mammalian cells, Golgi body is newly formed from assembly of small vesicles. We adopted dynamical triangulation method for coarse graining of membrane performed Monte-Carlo simulation to reproduce the Golgi organization process. We found that the control of membrane fusion based on local membrane structure is necessary to organize and maintain the fine Golgi-like shape. We also characterized the self-organization of fine Golgi-like shape via balances among three time scales of vesicle aggregation, membrane shape relaxation and membrane fusion.

標題：中性子セミナー：粉末中性子磁気構造解析の現状
日時：2017 年 1 月 17 日(火)　午後２時～午後３時
場所：物性研究所本館６階 第２セミナー室（A612）
講師：萩原 雅人
所属：物性研究所
要旨：

中性子回折法は磁性体の磁気構造決定において最も強力なツールである。従来数ミリオーダー以上の単結晶試料による弾性散乱測定により磁気構造が決定されてきたが、中性子線の出力や回折装置の高度化により微小単結晶でも解析できる十分なデータが得られるようになった。一方、結晶の方向の情報が失われる粉末試料においても、結晶の空間群の対称性を用いた磁気モデルの構築を利用することにより、磁気構造解析が結晶構造解析と同じく一般的なものになってきた。この背景には磁気既約表現によるモデリング[1]と、FullProf[2]や GSAS[3]等の Rietveld 粉末解析ソフト、VESTA[4]等の可視化ソフトとの密接な連携がある。最近では元の空間群との関係や、対称性と物理的性質のつながりを明確にする観点から、磁気空間群を用いた磁気モデルの構築が再評価されており、この支援環境も充実しつつある[5]。

本セミナーでは既約表現や磁気空間群による磁気構造解析の概要を示すとともに、実際にオークリッジ国立研究所の研究用原子炉 HFIR などで測定された回折実験のデータをもとに、各支援ソフトを用いた磁気構造解析例を示す。

備考：

[1] Y. A. Izyumov and V. E. Naish, J. Magn. Magn. Mater. 12, 239 (1979).
[2] J. Rodriguez-Carvajal, Physica B 192, 55 (1993).
[3] A.C. Larson and R.B. Von Dreele, Los Alamos National Laboratory Report LAUR 86-748 (2000).
[4] K. Momma and F. Izumi (2011): J. Appl. Crystallogr., 44, 1272-1276.
[5] M. I. Aroyo, J. M. Perez-Mato, D. et al., Bulg. Chem. Commun. 43(2) 183-197 (2011).

標題：ナノサイエンスセミナー：Heat-/Electron-/Light-/Force-induced tautomerization in a single porphycene molecule
日時：2017年1月17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：熊谷　崇
所属：フリッツ・ハーバー研究所
要旨：

Tautomerization in a single organic molecule is a fascinating model to study hydrogen dynamics and has recently obtained increasing attention in the field of nanoscale science because the process resembles a single-molecule switch. We have studied tautomerization of porphycene (a structural isomer of free-base porphyrin) by using low-temperature scanning probe microscopy (LT-SPM). Porphycene exhibits particularly interesting tautomerization behavior due to its strong intramolecular hydrogen bonds, and the investigation with LT-SPM opens a unique opportunity for studies of hydrogen-bond dynamics at the single-molecule level. I will discuss direct observation and control of tautomerization in the porphycene molecule on metal surfaces induced by different external stimuli-heat, tunneling electron, light, and force.

標題：ナノサイエンスセミナー：Machine learning to physics: extracting information from imaging and spectroscopic data in microscopy
日時：2017年1月20日(金)　午後1時30分～
場所：物性研究所本館6階 大講義室（A632）
講師：Dr. Rama K. Vasudevan
所属：Center for Nanophase Materials Sciences, Institute for Functional Imaging of Materials and Oak Ridge National Laboratory
要旨：

The past decade has seen enormous increases in the size and quality of datasets produced by techniques such as scanning probe microscopy and x-ray diffraction from synchrotrons globally. However, the necessary pathways to both mine the large datasets to derive understanding of fundamental mechanisms, as well as synthesize and compare the results across the wider available literature, are still generally limited. Here, I will present case studies involving our use of machine learning and deep data analysis of scanning probe microscopy datasets for understanding of physical mechanisms.

I will first outline the new suite of techniques that we have developed using scanning probe microscopy, which we term the "General mode" acquisition technique, that streams all of the information available from the measurement system (photodetector, current amplifier, etc.) to be captured and analyzed. This large increase in data volume allows for a wide variety of subsequent analysis, including data-driven filtering, digital lock-ins, and denoising. These techniques can greatly increase the acquisition speed by orders of magnitude for typical SPM experiments, such as in I-V curve acquisition on conductive oxides, and hysteresis loop acquisition for ferroelectrics.

Throughout the talk I will emphasize techniques to learn physics from the large datasets captured, including examples of endmember extraction, Bayesian inference, matrix factorization and convolutional neural networks that can be utilized to automatically learn appropriate features from images for classification, and from which subsequent physics is then derived by combining the information with first principles and thermodynamic models. These advances point to the big-data driven future of scanning probe microscopy as a vital tool for materials science researchers, as a means towards understanding local physics in complex material systems.

This work has been performed in collaboration with Suhas Somnath, Petro Maksymovych, Maxim Ziatdinov, Stephen Jesse, and Sergei V. Kalinin. The imaging and deep data analysis portion was sponsored by the Division of Materials Sciences and Engineering, BES, DOE. This research was conducted and partially supported at the Center for Nanophase Materials Sciences, which is a US DOE Office of Science User Facility.

標題：理論インフォーマルセミナー：First-principles design of magnetic topological insulators
日時：2017 年 1 月 20 日(金)　午後 3 時 30 分～午後 4 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：Max-Planck-Institut für Mikrostrukturphysik, Germany
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 quantised 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：第二回量子物質セミナー：Antiferromagnetic spintronics - spin-transfer torque and spin-motive force
日時：2017 年 1 月 27 日(金)　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：山根 結太
所属：The Institute of Physics at Mainz University
要旨：

Louis Néel, who received Nobel Prize in Physics 1970 for his pioneering work on magnetic properties of solids, commented in his Nobel lecture that "They (antiferromagnets) are extremely interesting from the theoretical viewpoint, but do not seem to have any applications." More than 40 years after his winning the prize, now antiferromagnets seem to be finally finding their major applications in the field of spintronics; people are realizing that replacing ferromagnets involved in spintronic devices by antiferromagnetic materials can lead to downsizing of the devices as well as much faster operations. One of the difficulties in dealing with antiferromagnetic materials, however, comes from the absence of macroscopic magnetization, making it hard to control them by magnetic fields. In this talk, we will discuss two phenomena, spin-transfer torque and spin-motive force, which could provide a route to generate and detect dynamical antiferromagnetic textures by electrical means.

標題：理論セミナー：Toward accurate description of surfaces and interfaces

日時：2017 年 1 月 27 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：Ikutaro Hamada

所属：Center for Green Research on Energy and Environmental Materials, National Institute for Materials Science

要旨：

Accurate description of complex systems including heterogeneous interfaces, such as molecule/metal and solid/liquid interfaces is important in diverse fields, e.g., heterogeneous catalysis, molecular electronics, and electrochemistry, but it poses a challenge on the electronic structure method as it requires the accurate description of the different interactions on the same footing. I will discuss the van der Waals density functional (vdW-DF) [1,2] as one of the efficient approaches to describe complex interfaces and show that by appropriate design of the exchange and correlation functionals [3], it is possible to accurately describe wide range of materials, including graphene on metal surfaces [4].

References

[1] M. Dion, H. Rydberg, E. Schroder, D. C. Langreth, and B. I. Lundqvist, Phys. Rev. Lett. 92, 246401 (2004).

[2] K. Lee, D. D. Murray, L. Kong, B. I. Lundqvist, D. C. Langreth, Phys. Rev. B 82, 081101(R) (2010).

[3] I. Hamada, Phys. Rev. B 89, 121103 (2014).

[4] F. Huttmann, et al, Phys. Rev. Lett. 115, 236101 (2015).

標題：ナノスケール-量子物質セミナー：二次元物質ファンデルーワルスヘテロ界面における 電子・光・スピン・超伝導制御

日時：2017 年 2 月 2 日(木)　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：守谷 頼

所属：東京大学生産技術研究所

要旨：

1原子層・1分子層の厚みでも安定に存在できる物質、それが二次元物質である。これらの物質は面直方向には結合手を持たないため、異なる物性、結晶構造、格子定数を持つ単結晶薄膜をファンデルワールス(vdW)力によって自由に積層した、vdW ヘテロ構造の実現が可能である。我々はこれまでに様々な vdW ヘテロ構造を作製し電子・光・スピン・超伝導分野との融合を目指してきた。

超伝導を示す二次元物質 NbSe2 同士を意図的にずらして積層させた vdW 接合においては超伝導体間の波動関数の結合が切れ、ジョセフソン電流が流れることを発見した。外部磁場による超伝導電流の位相変調に成功し、vdW 界面がジョセフソン接合として振る舞うことを見出した [1]。またグラフェン/NbSe2 構造においては、超伝導近接効果によりグラフェン内への超伝導ギャップの形成に成功した。

二次元の結晶構造はスピン依存伝導やスピン軌道相互作用の研究の場としても興味深い。我々は単原子層 h-BN トンネルバリアを介したスピン依存伝導や、グラフェンへのスピン注入、さらに二次元物質強磁性体とそのヘテロ構造の実現等の成果をもとに、二次元物質 vdW 界面におけるスピントロニクス技術の確立を目指している [2]。

グラフェンは状態密度が通常の金属と比べて極めて小さいため、グラフェン/MoS2 ヘテロ接合においては界面のショットキー障壁の伝導が外部電界により、ほぼ絶縁からオーミックまで大きく変調されることを示した [3]。

その他セミナーでは二次元物質の持つ様々な可能性と展望についても紹介する予定である。

参考文献

[1] N. Yabuki, R. Moriya et al., Nature Communications 7, 10616 (2016).

[2] T. Yamaguchi, R. Moriya et al., Appl. Phys. Express 6, 073001 (2013); M. Arai, R. Moriya et al., Appl. Phys. Lett. 107, 103107 (2015); T. Yamaguchi, R. Moriya, et al., Appl. Phys. Express 9, 063006 (2016).

[3] Y. Sata, R. Moriya, et al., Appl. Phys. Lett. 107, 023109 (2015); R. Moriya, et al., Appl. Phys. Lett. 106, 233103 (2015); T. Yamaguchi, R. Moriya, et al., Appl. Phys. Lett. 105, 223109 (2014); R. Moriya, et al., Appl. Phys. Lett 105, 083119 (2014); R. Moriya, et al., ECS Trans. 69, 357 (2015).

標題：Cathode lens electron microscopy
日時：2017 年 2 月 7 日(火)　午後 4 時～午後 5 時 30 分
場所：物性研究所本館 6 階 第 1 会議室（A636）
講師：Ernst Bauer
所属：Department of Physics, Arizona State University
要旨：

Cathode lens electron microscopy is a method for imaging surfaces and thin films with reflected or emitted low energy electrons. This talk will discuss the principles, possibilities and limitations of the various operation modes. They include the reflection modes low energy electron microscopy (LEEM) and mirror electron microscopy (MEM), the emission modes photo emission electron microscopy (PEEM) with UV, laser and synchrotron X-ray light excitation and Auger electron emission microscopy. Some of these operation modes give not only structural information but also magnetic information, making use of the spin dependence of the reflectivity or the circular dichroism in emission. Chemical information can be obtained with X-ray PEEM (XPEEM) and Auger electron emission microscopy (AEEM) via energy filtering. In addition to imaging most instruments allow also diffraction and spectroscopy. Combining several of these techniques a rather comprehensive characterization of surface and thin films on the 1 to 10 nm resolution level is possible, depending upon operation mode and instrument design. The ultimate resolution is limited by the long wavelength of low energy electrons to about 2 nm in aberration-corrected instruments.

The talk assumes familiarity with the basic physical processes involved in these imaging modes, such as electron diffraction, UV and X-ray photoelectron emission and Auger electron emission, in order to allow enough time for the illustration of their application with examples.

General reference: E. Bauer: Surface Electron Microscopy with Slow Electrons, Springer, New York, 2014

標題：理論セミナー：Rare-earth magnet
日時：2017 年 2 月 10 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：三宅　隆
所属：産業技術総合研究所、物質・材料研究機構
要旨：

Rare-earth magnets are mainly composed of 3d transition metals (T) and rare-earth metals (R). The former yield large magnetization, while the latter are a source of strong magnetocrystalline anisotropy (at low temperature). Strong magnet compounds, such as Nd2Fe14B and Sm2Fe17N3, contain a light element (X) as a third element. We will discuss the role of the X element in the magnetism of R-T-X systems. First-principles calculations [1] clarify that the magnetic moment depends sensitively on X as a consequence of orbital hybridization between X-2p and T-3d. Crystal-field coefficients at the R sites are also affected by X. This suggests that magnetocrystalline anisotropy can be controllable by additive elements. We will also present a combined first-principles and classical spin model analysis of magnetocrystalline anisotropy at finite temperature [2,3,4].

[1] Y. Harashima et al., Phys. Rev. B 92, 184426 (2015).
[2] M. Matsumoto et al., J. Appl. Phys. 119, 213901 (2016).
[3] Y. Toga et al., Phys. Rev. B 94, 174433 (2016).
[4] T. Fukazawa et al., arXiv:1612.04478.

標題：理論インフォーマルセミナー：Finite-temperature magnetism of 4f-3d intermetallics: a set of ab initio studies
日時：2017 年 2 月 24 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：松本 宗久
所属：東京大学物性研究所
要旨：

Rare-earth permanent magnets are important materials both technologically and scientifically. They are used in traction motors of hybrid vehicles and power generators to provide a sustainable solution to the energy problem. In those industrial applications, a recent challenge has been to soften a high-temperature degradation of the magnetic properties. Engineering of microstructure to better control the extrinsic properties has been pursued while we propose an intrinsic solution spotting a key energy scale of an exchange coupling between the anisotropic 4f-electron cloud in rare-earth atom and the magnetically polarized 3d-electron bands coming from the Fe-group elements. A simplified spin model derived basically from first principles shows that a slight enhancement of 4f-3d exchange coupling helps in partially avoiding the temperature degradation of the magnetic properties around the room temperature or higher [1]. Calculated temperature dependence of magnetic properties in our ab initio spin model is not entirely consistent with experimental results [1,2] of which reason can be at least partially tracked down to the fundamental issue in describing the nature of delocalized electrons on the basis of localized degrees of freedom. Other independent ab initio finite-temperature calculations for rare-earth permanent magnet compounds [3] provide a cross-check with ab initio description of itinerant electrons within Korringa-Kohn-Rostoker (KKR) method for the electronic structure calculation combined with coherent potential approximation (CPA) [4]. Finite-temperature scaling analysis between magnetization and uni-axial magnetic anisotropy energy elucidates the common nature and a difference between a spin model description, ab initio KKR-CPA, and the experimental results. Thus rare-earth permanent magnet makes a good playground for solid-state physics to address the nature of localized and itinerant magnetism. Extensions of the present models toward a finite-temperature description of magnetization reversal processes pose another challenge in statistical physics, and are under progress with several different approaches in implementing a scale-bridging scheme [5].

References
[1] MM, H. Akai, Y. Harashima, S. Doi, T. Miyake, J. Appl. Phys. 119, 213901 (2016).
[2] Y. Toga, MM, S. Miyashita, H. Akai, S. Doi, T. Miyake, A. Sakuma, Phys. Rev. B 94, 174433 (2016).
[3] MM, R. Banerjee, J. B. Staunton, Phys. Rev. B 90, 054421 (2014).
[4] H. Shiba, Prog. Theor. Phys. 46, 77 (1971); H. Akai, Physica 86-88B, 539 (1977).
[5] H. Sepehri-Amin, J. Thielsch, J. Fischbacher, T. Ohkubo, T. Schre, O. Guteisch, K. Hono, Act. Mater. 126, 1 (2017).

標題：凝縮系インフォーマルセミナー：Toward unified physics of quasi-one-dimensional organic superconductors: (TMTTF)2X in the metallic state (X=Br)
日時：2017 年 2 月 27 日(月)　午後 4 時～午後 5 時
場所：物性研究所本館 6 階 第 2 セミナー室（A612）
講師：Prof. Woun Kang
所属：Ewha Womans University, Seoul, Korea
要旨：

(TMTTF)2X is the sulfur analog of the well-known quasi-one-dimensional (Q1D) organic superconductor (TMTSF)2X and precedes it in the development of organic metals. Although they are metallic at room temperature, they undergo transitions into various insulating states at low temperature. While the insulating states deserved intensive study by themselves, efforts have been made to bring (TMTTF)2X to a metal at low temperature and to find superconductivity therein. Over a period of 14 years, superconductivity was confirmed in four members of (TMTTF)2X such as X=Br, PF6, AsF6, SbF6 under relatively high pressure. On the other hand, a generic phase diagram has been proposed to assume that the physics of the selenium and sulfur series must be treated on an equal footing. In an effort to support this idea, there has been a number of attempts to verify if the metallic state of (TMTTF)2X has indeed the same ingredients as those of (TMTSF)2X, but without much success until recently. In this study, we chose (TMTTF)2Br for a practical reason and studied the angular dependent magnetoresistance oscillations (AMRO) and the Hall effect under high pressure. Two of the most representative properties of Q1D metals, three-dimensional AMRO oscillations (including Lebed resonances, Danner-Chaikin oscillations, and the third angle effect) and field-induced spin-density-waves accompanied with quantized Hall resistance, were unambiguously confirmed in (TMTTF)2X in the end. These results suggest that physics of Q1D electronic system is universal regardless of the sulfur and selenium series.

標題：理論セミナー：Shot noise and Bell pair creation in nonlinear current of Kondo quantum dots
日時：2017 年 3 月 3 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：阪野　塁
所属：京大学物性研究所
要旨：

Low energy properties of the Kondo−correlated quantum dots are described by the local Fermi−liquid which is an extension of famous Landau’s Fermi−liquid to impurity systems where the Coulomb interaction works only for electrons in the impurity site. The non−equilibrium Kondo state has been intensively investigated in quantum dots, where non−equilibrium state is finely tuned and investigated by applying small bias−voltages between electric leads connected to the dot. A prominent result from the non−equilibrium Kondo effect is that residual interaction of the Fermi liquid generates quasiparticle pairs with 2e effective charge in nonlinear currents, and the pair can be observed as an enhancement of the shot noise.

We show theory and experiments on Fermi−liquid nature in shot noise measurement in a carbon nanotube quantum dot1−3. Particularly, current and noise due to the Kondo effect in carbon nanotube quantum dot where the local moment constituted of not only spin and but also chiral or orbital degrees of freedom emerges are discussed.
Furthermore, a new entangled−electron−pair generator utilizing the pair creation of the local Fermi−liquid in electric current in a quantum dot device is discussed. It is elucidated that local−Fermi−liquid exchange interaction violates

the Clauser–Horne–Shimony–Holt type Bell’s inequality for nonlinear currents through correlated two different channel of a double quantum dot device.

1. Ferrier, RS, *et al.*, Nat. Phys., **12**, 230–235 (2016).
2. Y Teratani, RS, *et al.*, J. Phys Soc. Jpn. **85**, 094718 (2016).
3. M Ferrier, RS, *et al.*, submitted to PRL.

標題：理論セミナー：On the dynamics of a 1D and 2D prototype quantum many body system
日時：2017 年 3 月 10 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：Xenophon ZOTOS
所属：ISSP, The University of Tokyo / University of Crete
要旨：

I will present recent results
(i) on a novel thermal Bethe ansatz approach to magneto-thermal transport in the Heisenberg spin 1/2 chain, as well as an extension to far out of equilibrium thermal transport (thermal quench) [1],
(ii) on the high temperature dynamics of quantum compass models [2].

References:

[1] X. Zotos, arXiv: 1604.08434
[2] A. Briffa and X. Zotos, arXiv: 1611.00637

標題：LASOR **セミナー：**Exploration of novel two-dimensional materials
日時：2017 年 3 月 21 日(火)　午前 10 時 30 分～
場所：物性研究所本館 6 階 第 1 会議室（A636）TV 会議（SPring-8 中央管理棟　3 階　TV 会議室）
講師：Dr. Baojie Feng
所属：東京大学物性研究所軌道放射物性研究施設　松田巌研究室
要旨：

During the last decade, two-dimensional (2D) materials, exemplified by the well-known graphene that can be exfoliated from the bulk phase, have attracted intensive attention. The advent of novel 2D materials makes it possible to fabricate devices at the atomic scale. Here, I will briefly introduce three of the newly emerging 2D materials: silicene, borophene and Cu2Si. These materials contain only one atomic layer and have been successfully synthesized on metal substrates by molecular beam epitaxy (MBE). Scanning tunneling microscopy (STM) and angle resolved photoemission spectroscopy (ARPES) measurements have unraveled intriguing properties in these materials, such as the Dirac cones in silicene and borophene and Dirac nodal lines in Cu2Si. These novel properties are not only of fundamental interest but also essential for the future device applications.