物性研究所セミナー

標題：第六回光量子融合連携研究開発プログラム進捗研究会「極限レーザーと先端放射光技術の融合による軟Ｘ線物性科学の創成」

日時：2016 年 6 月 3 日(金)　午後 1 時～

場所：姫路じばさんビル 4F　401 会議室

要旨：

近年の極限的なレーザー技術の革新により、極端紫外から軟Ｘ線にわたる短波長光の発生が実現し、放射光を補完する光源として期待されている。一方放射光における先端的な計測技術も着実に進展しており、X 線を用いた時間分解や顕微分光計測が可能となっており、今後は光源の垣根を越えたさまざまな利用法の開発が大きな課題となっている。本研究会は、平成 25 年度から文部科学省「光・量子融合連携研究開発プログラム」で採択された研究課題「極限レーザーと先端放射光技術の融合による軟Ｘ線物性科学の創成（課題責任者：辛埴）」に携わる研究グループによる進捗報告会であり、文化の異なるレーザーと放射光コミュニティ間の交流を通じてお互いの理解を深め、レーザーと放射光を共通基盤とした新しい物質科学の創成を目指す。

標題：理論セミナー：Schottky junctions studied using Korringa-Kohn-Rostoker non-equilibrium Green´s function method

日時：2016 年 6 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：赤井 久純

所属：東京大学物性研究所

要旨：

A scheme that combines the non-equilibrium Green's function method with the Korringa-Kohn-Rostoker (KKR) Green's function method is proposes. The method is different from most previous attempts [1-3] in that it uses the exact Green's function whose spectrum is not bound within a finite energy range, and hence, it provides sounder basis for quantitative discussions than the methods using the finite basis sets do. The scheme is applied to the Schottky junctions composed of a Al/GaN/Al trilayer.

Schottky contacts formed in metal/semiconductor junctions play an important role in semiconductor devices and integrated circuits [4]. They have been intensively investigated for several decades not only for possible application to electronic devices but also for gaining a fundamental understanding of the Schottky barrier formation.

Our results show that the Schottly barrier is formed between an undoped GaN and Al interface. The transport property of this system under various finite bias voltages is calculated. It is shown that the asymmetric behavior of electron transport against the direction of bias voltage occurs in this system, confirming the feature of rectification.

References

[1] J. M. Soler, E. Artacho, J. D. Gale, A. Garcia, J. Junquera, P. Ordejon, and D. Sanchez-Portal, J. Phys.: Condens. Matter 14, 2745 (2002).

[2] D. R. Bowler, T. Miyazaki, and M. J. Gillan, J. Phys.: ?Condens. Matter 14, 2781 (2002).

[3] T.Ozaki and H.Kino, Phys.Rev.B72,045121 (2005).

[4] S. M. Sze and K. K. Ng: *Physics of Semiconductor Devices* (John Willey and Sons, Hoboken, NJ, 2007).

標題：機能物性セミナー：固体高分子形燃料電池におけるカーボン系カソード触媒による酸素還元反応 −N ドープカーボンは遷移金属なしで酸素還元を促進するのか？−

日時：2016 年 6 月 16 日(木) 午前 11 時～

場所：第二会議室（TV 会議 SPring-8 会議室）

講師：難波江 裕太

所属：東京工業大学 物質理工学院材料系

要旨：

固体高分子形燃料電池(PEFC)の実用化において、電極触媒に用いられている白金のコスト、および希少性が、本格普及の妨げになっており、白金使用量の大幅低減を可能とする触媒が、切望されている。そこで近年、炭素、窒素を含む前駆体を少量の遷移金属と共に熱処理して得る、カーボン系カソード触媒が注目を集めている。本発表では、我々が最近取り組んでいる、鉄含有ポリイミド微粒子(Fe/PINP)由来のカーボン系触媒の開発状況と、共同研究者とともに取り組んでいるメカニズム研究について紹介する。

Reference

1. Y. Nabae et al., Sci. Rep., 6, 23276 (2016).
2. Y. Nabae et al., J. Mater. Chem. A, 2, 11561-11564 (2014).

標題：理論セミナー：超効率的なカオスモンテカルロ計算ー相関の可制御性と、物理計算への応用についてー

日時：2016 年 6 月 17 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：梅野 健

所属：京都大学大学院情報学研究科、 東京大学物性研究所

要旨：

全てのモンテカルロ計算法の基礎には、エルゴード性がある。が、一乱数の相関の特性によってその計算スピードは異なる。用いる乱数の相関が弱く、中心極限定理が成立する状況では、誤差分散が、計算ステップ数 N に対して O(1/N)となる通常の振る舞いをするが、相関が無視できない乱数を用いる場合、中心極限定理が成立しない状況ー誤差分散が O(1/N2)に収束する超効率的なモンテカルロ計算が可能であることーを、1998 年講演者によって発見された。その計算原理自体は、まだ新しく、一部の工学の分野（例：米国の携帯電話チップメーカーである Qualcomm 社の C-A. Yang , UCLA の Kung. Yao）で用いられてきたがメトロポリス法等のモンテカルロ法の本家となる物理分野では用いられてこなかった。

本講演では、その誤差分散が O(1/N2)となるメカニズムを、混合性を持つ乱数の相関の可制御性から説明し、物性理論分野の“新しい”超効率モンテカルロ計算法の構築につながるかという問題提起をし、議論したい。

標題：ナノサイエンスセミナー：ESR spectroscopy using nitrogen-vacancy centers in diamond
日時：2016 年 6 月 17 日(金)　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：高橋　晋
所属：南カリフォルニア大学、化学科
要旨：

Magnetic resonance (MR), such as nuclear magnetic resonance (NMR) and electron paramagnetic resonance (EPR), can probe the local structure and dynamic properties of various systems, making them among the most powerful and versatile analytical methods. However, their intrinsically low sensitivity precludes MR analyses of samples with very small volumes; e.g., more than 1010 electron spins are typically required to observe EPR signals at room temperature. A vast improvement in the current limits of MR will enable the imaging of structures and conformational changes of molecules in solution at the single molecule level.

A nitrogen-vacancy (NV) center in diamond is a promising candidate for applications in room temperature magnetic sensing with single spin sensitivity. In this presentation, we will discuss EPR spectroscopy using on NV centers in diamond. By employing EPR and double electron-electron resonance (DEER) techniques, we investigate impurities and coherence in diamond.1-3 We also demonstrate EPR of several electron spins using NV-based EPR spectroscopy. Moreover, we will discuss development of a high-frequency NV-based EPR system.4 This work is supported by NSF and the Searle Scholar program.

[1] F. H. Cho, ST et al., Rev. Sci. Instrum. 85, 075110 (2014).
[2] V. Stepanov and ST, arXiv:1603.07404.
[3] C. Abeywardana, ST, arXiv:1507.08744.
[4] V. Stepanov, ST et al., Appl. Phys. Lett. 106, 063111 (2015).

標題：第 38 回極限コヒーレント光科学セミナー「電子を用いた新しい水溶液計測法の開発とその応用」
日時：2016 年 6 月 23 日(木)　午後 2 時～午後 3 時
場所：物性研究所本館 6 階 第 1 会議室（A636）
講師：由井 宏治
所属：東京理科大学
要旨：

強いレーザーパルス光を水溶液中の物質に集光照射すると、物質は誘電破壊されプラズマ化する。発表者は、水溶液がプラズマへ相転移する前に溶液中に生み出された電子が、周囲の水分子の分極率の変化を誘起し、ラマン散乱断面積の 10^2～10^5 倍の増強を促すことを見出した。ラマンスペクトルは、分子の微視的構造や相互作用を鋭敏に反映するため、水溶液の微視的環境・物性の起源に関する情報を得ることができる。ラマン散乱分光法は水の強い赤外吸収に妨害されないため、発表者はこれらの特徴を活かして、これまで計測の難しかった様々な不均一系、また観測窓の限られる極限条件における水の微視的環境を明らかにしてた。また水溶液環境が重要となる生体・環境・様々な産業プロセスへの応用分析にも期待がもたれる。またレーザー誘起ではなく、最近の水溶液中電極間放電プラズマを用いた実験系についても紹介したい。

標題：理論インフォーマルセミナー：Local physical quantities for spin based on quantum electrodynamics
日時：2016 年 6 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：福田 将大
所属：東京大学物性研究所
要旨：

The local picture of electron spin is studied in the framework of quantum electrodynamics(QED).

In the framework of QED, one of the fundamental local physical quantities is the energy-momentum tensor density, which is derived from the general principle of relativity.

Recently, the “quantum spin vorticity theory” [1] is proposed as a consequence of the general relativistic symmetry of the energy-momentum tensor.

The quantum spin vorticity theory can give the time evolution equations of the electronic momentum density and the spin angular momentum density as equations which relate local mechanical physical quantities derived from the energy-momentum tensor density.

These local images of an electronic state by the quantum spin vorticity theory can help us to understand spin phenomena in condensed matter and molecular systems from a unified viewpoint [2,3].

[1] A. Tachibana, J. Math. Chem. 50, 669 (2012); Electronic Stress with Spin Vorticity. In Concepts and Methods in Modern Theoretical Chemistry, S. K. Ghosh and P. K. Chattaraj. Eds., CRC Press, Florida (2013), pp. 235-251; J. Comput. Chem. Jpn. 13, 18 (2014); Indian J. Chem. A, 53, 1031 (2014).
[2] M. Fukuda, K. Soga, M. Senami, A. Tachibana, Int. J. Quant. Chem., 116, 920 (2016).
[3] M. Fukuda, K. Ichikawa, M.Senami, A. Tachibana, AIP Advances 6, 025108 (2016).

標題：機能物性セミナー：液相界面での分子積み木細工によるナノシート結晶の創製
日時：2016 年 7 月 4 日(月)　午後 0 時 30 分～午後 1 時 30 分
場所：物性研究所本館 6 階 第 2 セミナー室（A612）
講師：牧浦 理恵
所属：大阪府立大学大学院工学研究科物質化学系専攻
要旨：

電子機器に対するより軽く・薄くといった社会的要求に加え、省資源化が望まれる中、ナノメートルスケールの厚みを有する 2 次元物質ナノシートは、究極に薄い機能材料として注目を集めている。有機分子を構成要素として得られる分子ナノシートは、構造設計性に優れ、多様なナノシートの創製が期待される。本セミナーでは、液相界面を用いた分子ナノシート結晶に関して、液面でのその場放射光 X 線回折測定により解明した形成過程、構造制御、光電子機能に関して講演する。

標題：新物質セミナー：Multiferroics by design with frustrated molecular magnets
日時：2016 年 7 月 6 日(水)　午後 1 時～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：紙屋 佳知
所属：理化学研究所
要旨：

Geometric frustration in Mott insulators permits perturbative electron fluctuations controlled by local spin configurations [1]. The simplest example is an equilateral triangle, “trimer”, of spins with S = 1/2, where low-energy degrees of freedom consist of built-in magnetic and electric dipoles arising from the frustrated exchange interaction. Such trimers, when weakly coupled, can be used to build multiferroics by design [2]. An organic molecular magnet known as TNN [3], with three S = 1/2 nitronyl nitroxide (NN) radicals in a perfect C3 symmetric arrangement, is an ideal building block, as was demonstrated by recent experiments on a single crystal comprising TNN and CH3CN. The fascinating thermodynamic phase diagram of this molecular crystal, TNN· CH3CN, is in excellent agreement with our theory, which predicts multiferroic behavior and strong magnetoelectric effects arising from an interplay between magnetic and orbital degrees of freedom [4]. Our study thus opens up new avenues for designing multiferroic materials using frustrated molecular magnets.

References:
[1] L. N. Bulaevskii, C. D. Batista, M. V. Mostovoy, and D. I. Khomskii, Phys. Rev. B 78, 024402 (2008).
[2] Y. Kamiya and C. D. Batista, Phys. Rev. Lett. 108, 097202 (2012).
[3] Y. Nakano et al., Polyhedron 24, 2147 (2005).
[4] Y. Kamiya et al., in preparation.

標題：LASOR **セミナー：規則合金における磁化ダイナミクスの制御とデバイス展開**
日時：2016 年 7 月 20 日(水)　午後 2 時 30 分～午後 3 時 30 分
場所：第一会議室（TV 会議　SPring-8 会議室）
講師：関　剛斎
所属：東北大学金属材料研究所
要旨：

異なる金属原子が規則的に空間配列した材料は規則合金と呼ばれ、実用材料として用いられている無秩序合金には無い優れた機能性を発現する。高い一軸磁気異方性を示す「L10 型 FePt 合金」、および伝導電子が高いスピン分極率を有する「L21 型ホイスラー合金」は磁性規則合金の一種であり、それらはナノサイズにおける磁化の高い熱安定性や磁気抵抗効果の増大をもたらすなど、スピントロニクスおよびナノマグネティクスが飛躍的な発展を遂げるためのキーマテリアルとなる。本セミナーでは、規則合金の磁気構造や磁化ダイナミクスを制御することによって、低い外部エネルギーで磁化反転を誘起できること[1,2]、また高周波自励発振を高性能化できること[3]を紹介する。ナノ磁性体における多様な磁化ダイナミクスを説明し、それらを理解する上で放射光を利用した精密評価の有用性についても議論したい。

[1] T. Seki et al., Nat. Commun., 4, 1726 (2013).
[2] T. Seki et al., J. Phys. D: Appl. Phys. 49, 075002 (2016).
[3] T. Seki et al., Appl. Phys. Lett. 105, 092406 (2014).

標題：機能物性セミナー「ヘムタンパク質の機能操作：超分子集合体および人工酵素の構築」
日時：2016 年 7 月 21 日(木)　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：大洞 光司
所属：大阪大学大学院工学研究科応用化学専攻
要旨：

ヘムタンパク質は、補因子としてポルフィリン鉄錯体（ヘム）を含み、生体内で物質変換の触媒や酸素貯蔵・輸送等の役割を担っています。我々のグループでは、ヘムを除去したヘムタンパク質に、化学的に合成した人工補因子を挿入し、ヘムタンパク質の機能改変を実施しています。本セミナーでは、天然のシステムに倣った人工酵素や光補集系および新規生体材料への応用を指向したヘムタンパク質集合体について紹介します。

文献 J. Am. Chem. Soc., 135, 17282-17285 (2013)、Chem. Commun., 51, 11138-11140 (2015).

標題：第 39 回極限コヒーレント光科学セミナー「テラヘルツ帯のエレクトロマグノン共鳴」
日時：2016 年 7 月 26 日(火)　午後 2 時~午後 3 時
場所：物性研究所本館 6 階 第 1 会議室（A636）
講師：高橋 陽太郎
所属：東京大学大学院工学系研究科
要旨：

誘電性と磁性が強く結びついているマルチフェロイクス物質中では、磁性に由来した強誘電性が出現する。マルチフェロイクス固有の素励起は、電気双極子遷移を伴うスピン波励起であり、エレクトロマグノンと呼ばれている。エレクトロマグノンは新しい素励起というだけではなく、励起状態内部の電気磁気結合効果を反映した電気磁気光学効果と呼ばれる新奇光学応答を示すことが明らかになってきた。本発表では、スピン構造や微視的な機構に基づいて、エレクトロマグノン共鳴において実現されている巨大な電気磁気光学効果や周辺の話題について紹介する。

標題：理論セミナー：Coarse-Grained Molecular Dynamics Simulation of Self-Assembled Macromolecules
日時：2016 年 8 月 4 日(木)　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：篠田　渉
所属：名古屋大学大学院工学研究科
要旨：

The talk illustrates recent development of our coarse-grained (CG) molecular model using a multi-property fitting approach. The CG model, known as the SDK CG model, is designed to reproduce experimental surface/interfacial properties as well as distribution functions from all-atom molecular dynamics (MD) simulations. This bottom-up approach to construct a CG model works well for lipids and surfactants self-assemblies, and has been extended to include proteins and polymers recently. This talk will particularly focus on zwitterionic phospholipid membranes, including vesicles. Membrane fusion and morphological changes of the lipid membranes are investigated in terms of free energy computation. A comparison of the CG-MD results with the conventional continuum model based on the Helfrich Hamiltonian elucidated non-trivial free energy contribution due to the conformational changes of lipids during the membrane deformation. The effects of the lipid components on the free energy barrier will be discussed. The effects of additives such as nanoparticles and peptides on the membrane properties will also be demonstrated.

標題：理論インフォーマルセミナー：第一原理電子状態計算を用いた新奇硫化物熱電材料の物性解明とマテリアルデザイン
日時：2016 年 8 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：宮田 全展
所属：北陸先端科学技術大学院大学 先端科学技術研究科
要旨：

熱電発電とはゼーベック効果を利用して熱エネルギーを電気エネルギーに変換する技術であり、密度の低い自然エネルギーや廃熱を用いて発電を行う“エネルギーハーベスティング”の中でも重要な位置を占めると期待されている。熱電発電素子として応用されている Bi_2Te_3 や PbTe は希少元素 Te を含むため、Te を含まない熱電材料の開発が求められている。同じ 16 族で地殻に豊富に存在する硫黄 S は Te の代替元素として有望であり、S を主成分とした硫化物熱電材料の研究が精力的に行われている。

我々は硫化物に注目し、第一原理電子状態計算と実験の両面から遷移金属硫化物ウルマナイト NiSbS が巨大な出力因子を示すことを明らかにした[1]。第一原理電子状態計算ソフトウェアパッケージ OpenMX[2]、ランダウアー理論に基づく電子輸送計算ツール QTWARE[3]を用いた詳細な電子構造の解析から NiSbS の高い出力因子の起源は化学ポテンシャル μ 近傍の擬ギャップ構造であることを明らかにした。本講演ではこれらの詳細について発表するとともに、第一原理電子状態計算を用いた新奇硫化物熱電材料のマテリアルデザインについても紹介する[4]。

[1] M. Miyata, T. Ozaki, S. Nishino, and M. Koyano, (submitted to J. J. Appl. Phys.).
[2] T. Ozaki, Phys. Rev. B **67**, 155108 (2003).
[3] http://www.rs.tus.ac.jp/takahiro/QTWare.html.
[4] M. Miyata, T. Ozaki, and M. Koyano, (submitted to J. Electron. Mater.).

標題：理論セミナー：Electromagnetic response of noncollinear antiferromagnets
日時：2016 年 8 月 31 日(水) 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：Dr. Hua Chen
所属：テキサス大学オースティン校
要旨：

In spite of rich properties and significant academic interest, antiferromagnets have always been overshadowed by ferromagnets in real-life applications based on magnetism, including spintronics. This is primarily due to the fact that antiferromagnet order parameter couples weakly to external magnetic field and has therefore been difficult to manipulate. In this talk I will discuss a number of recent theoretical and experimental developments that counter this conventional wisdom in a class of antiferromagnets with stable noncollinear magnetic order. As an introduction I will talk about the surprising discovery of the anomalous Hall effect (AHE), the generation of a voltage perpendicular to current in the absence of a magnetic field, in noncollinear antiferromagnets. In these materials the AHE can be used as an efficient probe to determine the global orientation of the noncollinear antiferromagnetic order. I will then discuss the coupling between the noncollinear order parameter and external electric and magnetic fields. Electric fields or currents can change the magnetization direction and induce collective dynamics through current- or electric-field-induced spin-orbit torques. I will show through both toy model and first principles calculations that the spin-orbit torque is nonzero in a prototypical noncollinear antiferromagnet, Mn_3Sn, in spite of its global inversion symmetry. As for external magnetic fields, although their direct coupling with noncollinear spin magnetization is rather weak, I will show that there is a large orbital moment in these noncollinear antiferromagnets. Coupling between the external

magnetic field and the orbital moment can lead to a torque on the noncollinear order parameter through a response function that can be viewed as dual to the current-induced torque.

標題：ナノサイエンスセミナー：Cryogenic variable temperature SP-STM study of perovskite-clad FeAs monolayers

日時：2016 年 8 月 31 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：Prof. Jhinhwan Lee

所属：Department of Physics, KAIST, Korea

要旨：

I. Plaquette antiferromagnetic order coexisting with iron superconductivity

The symmetry requirement and the origin of magnetic orders coexisting with superconductivity have been strongly debated issues of iron-based superconductors (FeSCs). Observation of C_4-symmetric antiferromagnetism in violation of the inter-band nesting condition of spin-density waves in superconducting ground state will require significant change in our understanding of the mechanism of FeSC. The superconducting material Sr_2VO_3FeAs, a bulk version of monolayer FeSC in contact with a perovskite layer with its magnetism (T_N ~ 50 K) and superconductivity (T_C ~ 37 K) coexisting at parent state, has no reported structural orthorhombic distortion and thus makes a perfect system to look for theoretically expected C_4 magnetisms. Based on variable temperature spin-polarized scanning tunneling microscopy (SPSTM) with newly discovered imaging mechanism that removes the static surface reconstruction (SR) pattern by fluctuating it rapidly with spin-polarized tunneling current, we could visualize underlying C_4 symmetric (2x2) magnetic domains and its phase domain walls coexisting with superconductivity. We find that this magnetic order is perfectly consistent with the plaquette antiferromagnetic order in tetragonal Fe spin lattice expected from theories based on the Heisenberg exchange interaction of local Fe moments and the quantum order by disorder. The inconsistency of its modulation Q vectors from the nesting condition also implies that the nesting-based C_2 symmetric magnetism is not a unique prerequisite of high-Tc FeSC. Furthermore, the plaquette antiferromagnetic domain wall dynamics under the influence of small spin torque effect of spin-polarized tunneling current are shown to be consistent with theoretical simulation based on the extended Landau-Lifshitz-Gilbert equation. (ArXiv:1608.00884, under review in Nat. Mat.)

II. Enhancement of superconductivity by interfacial phonons

The physics at the interface between monolayer iron-based superconductor (FeSC) and perovskite substrate has received considerable attention due to the unusually high Tc of ~100 K found recently in monolayer FeSe on $SrTiO_3$ substrate. It has been suggested that forward-scattering interfacial phonons coupled with the Fe-layer electrons can enhance superconductivity from almost any kind of pre-existing electron-based pairing, initiating the quest for perovskite-clad FeSC monolayer and its bulk heterostructure with higher coupling efficiency with interfacial phonons. Here we report a spectroscopic imaging scanning tunneling microscopy (SI-STM) study on a parent-compound superconductor Sr_2VO_3FeAs, the only currently known self-assembled bulk example of FeSC monolayers on perovskite layers with substantially high T_C ~ 37 K. It shows clear signatures of forward-scattering phonons with unprecedentedly strong coupling close to 1 probably due to doubled interfaces per FeSC monolayer. Our masked quasiparticle interference (QPI) analysis based on the superconducting gap map and the V-Fe hybridization strength map shows clear positive correlations between all pairs, which is the hallmark of pairing enhancement due to electron-phonon coupling with interfacial phonons. With the possibility of massive number of parallel superconducting layers

and the stronger electron-phonon coupling achieved, perovskite-clad FeSC monolayers may become a building block of the next generation Fe-based high-Tc superconductors with significantly enhanced Tc and current carrying capacity. (ArXiv:1608.00886, under review in Nat.)

標題：頭脳循環 ワークショップ "Frontier of Quantum Material Science and Nano-Technology"
日時：2016 年 9 月 5 日(月) 午前 10 時～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）
要旨：10:00-11:00

講師：Hua Chen (**テキサス大学オースティン校**)
標題：Orbital moments and current-induced magnetization dynamics in noncollinear antiferromagnets
要旨：

Now that the anomalous Hall effect is established as a convenient order parameter probe in a class of noncollinear antiferromagnets, it is timely to examine effects that can be used for order parameter manipulation. In this talk I will discuss some of our recent theoretical results on the coupling between the noncollinear magnetic order parameter and external electric and magnetic fields. First I will briefly explain the physics of orbital magnetic moments which arise from the coupling between magnetic fields and the orbital motion of electrons. A nonzero orbital moment is present in all ferromagnets, but is usually much smaller than the total spin moments. In noncollinear antiferromagnets like Mn3Ir or Mn3Sn, which have an anomalous Hall effect, sizable orbital moments exist while the total spin moment nearly vanishes. This orbital moment can be used to manipulate the order parameter using magnetic fields. Separately, in certain noncollinear antiferromagnets with broken atomic-site-inversion symmetry, a nonzero site-dependent spin polarization can be induced by external electric fields or currents, which can exert a torque on the local spin moments and can potentially change the direction of the noncollinear magnetic order parameter or induce its nontrivial dynamics.

11:00-12:00
講師：野村 健太郎（東北大学金属材料研究所）
標題：Spin-electromagnetic responses in topological matters
要旨：

The electrical control of spin magnetization aims to be used in next-generation magnetic devices, allowing information to be written electronically. Recently, spintronics phenomena in topological materials have been drawn interests for achieving novel electrical manipulation of the magnetization, and generation of spin currents. In this presentation we discuss theoretical proposals of spintronics phenomena in topological insulators and magnetic Weyl semimetals.

In the first part of the talk, spin-electricity conversion at the interface between a ferromag-netic material and a topological insulator[1] is discussed. Injected spins by spin pumping are converted into a charge current due to spin-momentum locking on the surface state. We for-mulate a theoretical model for spin dynamics and the spin-electricity conversion effect on the topological surface. The dumping constant is expressed in terms of the conductivity of the surface Dirac fermions. The electrically induced spin current is calculated using the perturba-tion theory.

In the second part, we discuss spintronics phenomena in magnetic Weyl semimetals. A Weyl semimetal is a new type of topologically protected gapless quantum state, with either time-reversal or spatial inversion symmetries broken in three dimensions. Weyl semimetals with broken time-reversal symmetry are more interesting and rewarding for spintronics applications. We derive an effective free energy functional of

magnetization which describes low energy excitations and magnetic textures[2]. We also demonstrate that Weyl electrons in a magnetically doped Weyl semimetal exert a spin torque on the local magnetization, without a flowing current, when the chemical potential is modulated in a magnetic field. The spin torque is proportional to the anomalous Hall conductivity, and its effective field strength may overcome the Zeeman field. Using this effect, the direc-tion of the local magnetization is switched by gate control in a thin film. We also discuss dynamics of local magnetization by solving the Landau-Lifshitz-Gilbert equation.

[1] Y. Shiomi, K. Nomura, Y. Kajiwara, K. Eto, M. Novak, K. Segawa, Y. Ando, E. Saitoh, Phys. Rev. Lett. 113, 196601 (2014).
[2] K. Nomura and D. Kurebayashi, Phys. Rev. Lett. 115, 127201 (2015).
[3] D. Kurebayashi and K. Nomura, arXiv:1604.03326.

13:30-14:30
講師：Lucile Savary（**マサチューセッツ工科大学**）
標題：Disorder-induced entanglement in spin ice pyrochlores
要旨：

I will discuss a proposal according to which, in a certain class of magnetic materials, known as non-Kramers 'spin ice,' disorder induces quantum entanglement. Instead of driving glassy behavior, disorder provokes quantum superpositions of spins throughout the system, and engenders an associated emergent gauge structure and set of fractional excitations. More precisely, disorder transforms a classical phase governed by a large entropy, classical spin ice, into a quantum spin liquid governed by entanglement. As the degree of disorder is increased, the system transitions between (i) a "regular" Coulombic spin liquid, (ii) a phase known as "Mott glass," which contains rare gapless regions in real space, but whose behavior on long length scales is only modified quantitatively, and (iii) a true glassy phase for random distributions with large width or large mean amplitude. These results may be applicable to Pr2Zr2O7, in which random crystal field splittings have already been observed, and to classical spin ices, such as Ho2Ti2O7, upon chemical doping.

標題：ナノサイエンスセミナー：Nanogap-Enhanced Raman Scattering (NERS)
日時：2016 年 9 月 7 日(水)　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. Yung Doug SUH
所属：Korea Research Institute of Chemical Technology (KRICT) and SungKyunKwan University
要旨：

Started from the simple wet-chemical nanogap generation induced by Coulomb aggregation among colloidal nanoparticles in aqueous solution after adding salt onto it shown independently by S. Nie and K. Kneipp in 1997, nanogap engineering to enhance Raman scattering signal to achieve single molecule sensitivity is getting more sophisticated. In this talk, single molecule Surface-Enhanced Raman Scattering (smSERS) field formed since 1997 will be briefly reviewed and then different types of nanogap engineering strategy for smSERS developed in my lab will be discussed: single-junction 0-D external nanogap between two spherical nanoparticles connected with a double helix DNA (Nature Materials 2010), multi-junction 3-D spherical nanogap internally formed between spherical gold core nanoparticle and spherical gold shell nanoparticle connected by multiple single helix DNAs (Nature Nanotech. 2011), and 2-D nanogap arrays formed on a 4-inch polymer wafer by simple two-step process. Several reasons will be

discussed why now SERS regime and NERS (Nanogap-enhanced Raman Scattering) regime should be separated on the enhancement factor (EF) distribution histogram. Recent result including direct near-field visualization of the nanogap field of the 2-D nanogap array, single molecule behavior of cytochrome C protein's Raman signal, and ultra-uniform distribution of SERS enhancement factor (EF) of benzene thiol molecule dispersed on this plasmonic 2-D nanogap array wafer will be presented.

List of Publications Related to this Presentation

1. D. Lim, K.-S. Jeon, H.M. Kim, J.-M. Nam, and Y.D. Suh, Nature Materials 9, 60 (2010)
2. D. Lim, K.-S. Jeon, J.H. Hwang, H.Y. Kim, S.H. Kwon, Y.D. Suh, and J.-M. Nam, Nature Nanotechnology 6, 452 (2011)
3. H. Lee, J.-H. Lee, S.M. Jin, Y.D. Suh, and J.M. Nam, Nano Letters, 13, 6113 (2013)
4. H. Lee, G.-H. Kim, J.-H. Lee, N.H. Kim, J.-M. Nam, and Y.D. Suh, Nano Letters, 15, 4628 (2015)
5. Y.I. Park, J.H. Kim, K.T. Lee, K.S. Jeon, H.B. Na, J.H. Yu, H.M. Kim, N. Lee, S.H. Choi, S.-I. Baik, H. Kim, S.P. Park, B.-J. Park, Y.W. Kim, S.H. Lee, S.-Y. Yoon, I.C. Song, W.K. Moon, Y.D. Suh, and T. Hyeon, Adv. Mater. (2009)
6. S.H. Nam, Y.M. Bae, Y.I. Park, J.H. Kim, H.M. Kim, J.S. Choi, K.T. Lee, T. Hyeon, and Y.D. Suh, Angewandte Chemie 50, 6093 (2011)
7. J.-W. Oh, D.-K. Lim, G.-H. Kim, Y.D. Suh, and J.-M. Nam, JACS 136, 14052 (2014)
8. H.J. Seo, S.H. Nam, H.-J. Im, J.-Y. Park, J.Y. Lee, B. Yoo, Y.-S. Lee, J.M. Jeong, T. Hyeon, J. W. Kim, J.S. Lee, I.-J. Jang, J.-Y. Cho, D.W. Hwang, Y.D. Suh, and D.S. Lee, Sci. Report, 5, 15685 (2015)
9. H.S. Park, S.H. Nam, J.W. Kim, H.S, Shin, Y.D. Suh, and K.S. Hong, Sci. Report, 6, 27407 (2016)

標題：新物質・理論インフォーマルセミナー：Targeted Synthesis of Hybrid Metal Organic Spin Liquids
日時：2016 年 9 月 9 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：Danna Freedman, T. David Harris
所属：ノースウェスタン大学
要旨：

Confining magnetic properties to two dimensions offers tremendous potential for the discovery of new properties. One intriguing possibility is creating a spin liquid whereby an infinitely degenerate magnetic ground state enables the realization of new quasiparticles.

Synthetic inorganic chemistry is the ideal vector by which to design spin liquids. Specifically we are targeting two dimensional kagome lattices, a structure predicted to house spin liquids. Danna Freedman will present prior results on the known spin liquid herbertsmithite, and Dave Harris will present a synthetic vision and progress towards the realization of a hybrid metal-organic spin liquid.

標題：理論インフォーマルセミナー：Field theory for symmetry protected topological properties of AKLT-type VBS states

日時：2016 年 9 月 20 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：高吉 慎太郎

所属：ジュネーヴ大学

要旨：

Mapping from quantum antiferromagnets to a semiclassical field theory such as nonlinear sigma models with topological terms has contributed insights into the nontrivial behavior of quantum fluctuations since the work by Haldane in 1980's. Recently, another aspect of AKLT states is focused, i.e., short-range entangled state protected by some symmetry. We explain how such symmetry protected topological (SPT) properties in AKLT-type VBS states are described using an effective field theory in spatial dimensions one through three.

Starting from the well-understood case of one-dimensional antiferromagnets and thereby establishing its validity, we proceed to the two-dimensional square lattice. Through a path integral representation of the ground state wave functional,we conclude that the ground state is an SPT state for the spin quantum number equal to two times odd integer while it is topologically trivial for two times even integer.

We also show that this representation of the ground state wave functional is closely related with the strange correlator,which is proposed as an indicator of SPT phase. Finally, we discuss generalization of the preceding approach to the case of a cubic lattice.

標題：理論セミナー：Emergence of negative capacitance in multi-domain ferroelectric thin film capacitors under bias

日時：2016 年 9 月 30 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：笠松 秀輔

所属：東京大学物性研究所

要旨：

In recent years, several experimental works have shown that “negative capacitance” can be attained in a ferroelectric thin film placed in series with a paraelectric [1]. To explain this, they claim that the negative capacitance is realized by suppression of spontaneous polarization in the ferroelectric due to the depolarizing effect coming from the paralectric film. However, such explanation has been criticized due to the fact that any such depolarizing effects are usually cancelled in ferroelectric materials through the formation of polarization domains.

In this talk, I will try to present a more convincing explanation of the mechanism for negative capacitance based on first-principles simulation results of a multidomain ferroelectric-paraelectric bilayer capacitor under bias voltage [2]. The finite-voltage simulations are performed using the orbital-separation approach [3] within the Kohn-Sham formalism of density functional theory. We show that domains evolve in an antiferroelectric-like way, and that negative capacitance can emerge as a result of monodomain formation under bias.

Reference:

[1] G. Catalan, D. Jiménez, A. Gruverman, Nature Mater. 14, 137 (2015).

[2] S. Kasamatsu, S. Watanabe, C. S. Hwang, and S. Han, Adv. Mater. 28, 335 (2016).

[3] S. Kasamatsu, S. Watanabe, and S. Han, Phys. Rev. B 84, 085120 (2011); Phys. Rev. B 92, 115124 (2015).