# 物性研究所セミナー

**標題：理論セミナー：**Fracture process of semicrystalline polymers in molecular scale by coarse-grained molecular dynamics simulation
**日時：**2016 年 1 月 8 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：**樋口 祐次
**所属：**東北大学金属材料研究所
**要旨：**

One of the big challenges by molecular theory is understanding the fracture process of semicrystalline polymers, which is important to increase toughness of polymeric materials in industry. The fracture process against the stretching is also tempting in physics because semicrystalline polymers show inhomogeneous structure and the process takes non-equilibrium pathway. In my talk, the fracture process of polyethylene is studied by coarse-grained molecular dynamics simulation. Lamellar layer, which consists of amorphous and crystal parts and is basic structure of polyethylene in molecular scale, is stretched parallel and perpendicular to the crystal direction. In the stretching process, recrystallization of grain boundary, fragmentation of lamellar structure, and tilt of crystal part are observed. Dynamics of polymer chains in molecular scale are successfully revealed.

**標題：中性子セミナー：**Macromolecular Translocation through Nanopores
**日時：**2016 年 1 月 19 日(火)　午後 2 時～午後 4 時
**場所：**物性研究所 6 階 第 6 セミナー室（A616）
**講師：**Prof. M. Muthukumar
**所属：**University of Massachusetts Amherst
**要旨：**

The ubiquitous phenomenon of translocation of electrically charged macromolecules through narrow pores exhibits bewildering phenomenology, requiring an adequate description of polyelectrolyte dynamics, electrolyte dynamics, hydrodynamics, and confinement effects from charge-decorated pores. The translocation process involves three major stages: (a) approach of the macromolecule towards the pore, (b) capture/recognition of the macromolecule at the pore entrance, and (c) threading through the pore. All of these stages are controlled by conformational entropy of the macromolecule, charge decoration and the geometry of the pore, hydrodynamics, and electrostatic interactions. Challenges in developing a unified theory of these contributing factors will be described in the context of a few illustrative experimental data on transport of DNA, proteins, and synthetic macromolecules through protein pores and solid-state nanopores.

**標題：第２回元素戦略プロジェクト<研究拠点形成型>／大型研究施設連携シンポジウム –局所構造制御で物質から材料へ–**
**日時：2016 年 1 月 21 日(木)～2016 年 1 月 22 日(金)**
**場所：伊藤国際学術研究センター（東京大学本郷キャンパス）**
**講師：神谷利夫（東京工業大学）、中村哲也（JASRI/SPring–8） 他**
**所属：上記の通り**
**要旨：**

本シンポジウムは、元素戦略プロジェクトに代表される物質科学研究の推進において、我が国が持つ世界に例のない大型研究施設・大型計算機の連携・協力による産官学コミュニティ全体の研究活動を促進し、顕著な成果を創出することを目標として、下記３点の議論・情報共有の場を提供いたします。

１．元素戦略の研究領域を題材とした、これまでの成果と大型研究施設の活用方法
２．元素戦略の視点から産業の先端ニーズとアカデミアの先端シーズ
３．課題解決の加速のために物質科学とデータ科学の連携の在り方

**標題：理論インフォーマルセミナー：**Spin liquids on kagome lattice and symmetry protected topological phase
**日時：2016 年 1 月 27 日(水) 午後 4 時 30 分～午後 5 時 30 分**
**場所：物性研究所本館 6 階 第 5 セミナー室（A615）**
**講師：**Yin Chen He
**所属：マックスプランク複合系物理研究所**
**要旨：**

In my talk I will introduce the spin liquid phases that occur in kagome antiferromagnets, and discuss their physical origin that are closely related with the newly discovered symmetry protected topological phase (SPT). I will first present our numerical (DMRG) study on the kagome XXZ spin model that exhibits two distinct spin liquid phases, namely the chiral spin liquid and the kagome spin liquid (the groundstate of the nearest neighbor kagome Heisenberg model). Both phases extend from the extreme easy-axis limit, through SU(2) symmetric point, to the pure easy-plane limit. The two phases are separated by a continuous phase transition. Motivated by these numerical results, I will then focus on the easy-axis kagome spin system, and reformulate it as a lattice gauge model. Such formulation enables us to achieve a controlled theoretical description for the spin liquid phases. We then show that the chiral spin liquid is indeed a gauged U(1) SPT phase. On the other hand, we also propose that the kagome spin liquid is a critical spin liquid phase, which can be considered as a gauged deconfined critical point between a SPT and a superfluid phase.

**標題：理論セミナー：**Fermionic spinon and holon statistics in the pyrochlore quantum spin liquid
**日時：2016 年 1 月 29 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 2 セミナー室（A612）**
**講師：**Bruce Normand
**所属：中国人民大学**
**要旨：**

We prove that the insulating one-band Hubbard model on the pyrochlore lattice contains, for realistic parameters, an extended quantum spin-liquid phase. This is a three-dimensional spin liquid formed from a highly degenerate manifold of dimer-based states, which is a subset of the classical dimer coverings obeying the ice rules. It possesses spinon excitations, which are both massive and deconfined, and on doping it exhibits spin-charge separation. We demonstrate that the spinons have fermionic statistics, and further that the holons introduced by doping are also fermions. We explain the origin of this counterintuitive result and establish the connection of these emerging fermions with U(1) gauge fields, represented by strings, as anticipated by Levin and Wen.

**標題：第 36 回極限コヒーレント光科学セミナー：Observation of Weyl fermions in condensed matter**
**日時：2016 年 2 月 9 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）**
**講師：Prof. Hong Ding**
**所属：Institute of Physics, Chinese Academy of Sciences**
**要旨：**

In 1929, a German mathematician and physicist Hermann Weyl proposed that a massless solution of the Dirac equation represents a pair of new type of particles, the so-called Weyl fermions. However, their existence in particle physics remains elusive after more than eight decades, e.g., neutrino has been regarded as a Weyl fermion in the Standard Model until it was found to have mass. Recently, significant advances in topological materials have provided an alternative way to realize Weyl fermions in condensed matter as an emergent phenomenon. Weyl semimetals are predicted as a class of topological materials that can be regarded as three-dimensional analogs of graphene breaking time reversal or inversion symmetry. Electrons in a Weyl semimetal behave exactly as Weyl fermions, which have many exotic properties, such as chiral anomaly, magnetic monopoles in the crystal momentum space, and open Fermi arcs on the surface. In this talk I will report our experimental discovery of a Weyl semimetal in TaAs by observing Fermi arcs with a characteristic spin texture in the surface states and Weyl nodes in the bulk states using angleresolved photoemission spectroscopy.

**標題：理論インフォーマルセミナー：Bootstrapping controversial phase transitions**
**日時：2016 年 2 月 10 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：大槻 知貴**
**所属：カブリ数物連携宇宙研究機構**
**要旨：**

Recently the conformal bootstrap program has turned out to be a quite powerful way to study d>2 conformal field theories (CFTs) in a completely non-perturbative fashion. Indeed the "solution" obtained by the method offers the most precise estimate for the 3d Ising model critical exponents. In this talk, I will discuss the application of the bootstrap program to more controversial yet physically important problems, namely, the d=3 O(n)xO(2) symmetric Landau-Ginzburg models.

These models realize wide variety of physical systems at criticality, including anti-ferromagnetic spin systems placed on triangular lattices and 2-flavor QCD chiral phase transition (provided the axial anomaly is negligible). Despite their obvious physical relevance, the study of their renormalization group (RG) flow are notoriously hard and there are serious controversies over the nature of their phase transitions: depending on the methods (e.g. perturbative RG series, functional RG equation, lattice Monte-Carlo, etc) one obtains different result regarding the presence of IR-stable fixed points.

I will propose the resolution of this long-standing controversies using the conformal bootstrap program, based on our papers arXiv:1404.0489 and arXiv:1407.6195 with Yu Nakayama.

**標題：理論セミナー：G0W0 近似の妥当性と密度汎関数理論の基本思想**
**日時：2016 年 2 月 12 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：高田 康民**
**所属：東京大学物性研究所**
**要旨：**

ごく最近、超伝導転移温度 Tc の第 1 原理からの計算手法に関連してレビュー的な論文(過去の仕事のレビューから出発して一部に新しい結果や考察を含むもの)を 3 編出版した[1-3]。その際、ヘディンの自己無撞着な GW 近似に比べてそのワンショット版(いわゆる G0W0 近似)の方が実験との比較でより妥当な結果を与えるとの報告が 1980 年代から絶縁体・半導体で多数あり、また、近年では原子・分子系でより精密な計算に基づいて同様の議論が屡々なされているという事実を受け止めて、正常状態、及び、超伝導状態について G0W0 近似の妥当性を解析的・数値計算的に再考察した。その結果、ワード恒等式が重要な役割を果たす準粒子の分散関係や Tc のようなある種の物理量の計算に関しては、自己エネルギー補正とバーテックス補正の相殺効果によって、バーテックス補正が全く含まれない GW 近似よりも G0W0 近似の方が(バーテックス補正を暗黙裏に含んでいることから)より妥当であることが分かった。もちろん、全ての物理量が G0W0 近似で妥当に評価されるわけではない。

ところで、G0W0 近似では一体近似の情報から直接的に多体系の物理量が評価されるが、これは密度汎関数理論(DFT)の基本思想にも通じる。そこで、この観点から、グリーン関数法と DFT の関連を見つめ直し、DFT の時間依存版(TDDFT)や超伝導版(SCDFT)に現れる基本的な物理量(すなわち、交換相関核や対相互作用)の基本的な性質について見直すと同時に、その具体的な汎関数形を考察する。

[1] YT, “Role of the Ward identity and relevance of the G0W0 approximation in normal and superconducting states”, arXiv: 1601.02364; published online in Molecular Physics: DOI: 10.1080/00268976.2015.1131860.
[2] YT, “Theory of superconductivity in graphite intercalation compounds”, arXiv: 1601.02753; published in Reference Module in Materials Science and Materials Engineering (Saleem Hashmi; editor-in-chief), Oxford, Elsevier, 2016, ISBN: 978-0-12-803581-8; DOI: 10.1016/B978-0-12-803581-8.00774-8
[3] YT, “Theory for reliable first-principles prediction of the superconducting transition temperature”, arXiv: 1601.03486; published in Carbon based superconductors: Toward high-Tc superconductivity (edited by J. Haruyama), Pan Stanford, Singapore, 2015, pp. 193-230; ISBN: 978-981-4303-30-9 (Hardcover), 978-981-4303-31-6 (eBook).

**標題：理論インフォーマルセミナー：Spontaneous increase of magnetic flux and chiral-current reversal in bosonic ladders: Swimming against the tide**
**日時：2016 年 2 月 17 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：Dr. Teimuraz Vekua**
**所属：Leibniz University of Hannover, Institute of Theoretical Physic**
**要旨：**

The interplay between spontaneous symmetry breaking in many-body systems, the wave-like nature of quantum particles and lattice effects produces an extraordinary behavior of the chiral current of bosonic particles in the presence of a uniform magnetic flux defined on a two-leg ladder. While non-interacting as well as strongly interacting particles, stirred by the magnetic field circulate in the ground state along the system's boundary in the counterclockwise direction, interactions can stabilize states with broken translational symmetry, in which the circulation direction can be reversed. For the Bose-Hubbard model on the two-leg ladder, the states with spontaneously broken translational symmetry are vortex lattices that we have observed numerically. The current reversal survives up to temperatures that are already achieved in experiments on ultra-cold gases.

**標題：理論インフォーマルセミナー：First-principles design of magnetic materials**
**日時：2016 年 2 月 25 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：Dr. Arthur Ernst**
**所属：Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany**
**要旨：**

Nowadays first-principles methods enable quantitive and qualitative description of complex materials. Based on quantum mechanics and numerical methods, they are widely applied to study structural, electronic, magnetic, transport and optical properties of condensed matter without or almost without adjustable parameters.

In my talk I'll present one of such approaches, based on the multiple scattering theory using a Green function formalism. This method is designed to study bulk materials, surfaces, interfaces, clusters and alloys.
The main focus of our activity is magnetism and I'll show most prominent examples of our research in this field. After a very short introduction about the method, we use, I'll discuss how theoretical simulations of XAS & XMCD spectra can help to obtain adequate information about the chemical composition, structural, electronic and magnetic properties of complex materials such as magnetic oxides and otological insulators.

In the second part of my talk, I'll present a first-principles formalism to study spin waves. Spin waves or magnons are collective magnetic excitations, which provide important information about magnetic properties of solids.
Apparently, magnons participate in many physical phenomena such as superconductivity, domain wall motion, spin Seebeck effect etc. They can be described as quasiparticles of a certain wave vector and of a certain energy.
The wave vector and the energy are linked together by a characteristic dispersion relation. Spin waves can be studied with several experimental techniques such as ferromagnetic resonance, Brillouin light scattering, neutron scattering, scanning tunnelling and spin polarised electron energy loss spectroscopy.
Thereby, spin waves can be described theoretically using either a macroscopic phenomenological model or a microscopic treatment of solids. In my talk, I'll present a first-principles approach to calculate spin waves in complex systems such as bulk materials, surfaces and interfaces with and without disorder. The approach is based on a microscopic treatment of solids and implemented using a Green function method within the density functional theory.
The efficiency of our method will be illustrated through the comparison with recent experiments on bulk materials and thin films.

**標題：理論セミナー：多軌道電子系における局所磁気モーメント形成とスピン三重項超伝導**
**日時：2016 年 2 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：星野 晋太郎**
**所属：東京大学大学院 総合文化研究科**
**要旨：**

同じスピンを持つ電子が対形成したスピン三重項超伝導は、$Sr_2RuO_4$ や U 化合物を含む物質群においてその実現可能性が提案されている。通常、スピン三重項超伝導に対しては空間的に奇パリティ(p 波)をもつ異方的な電子対が仮定されるが、電子の持つ軌道自由度を考慮するならば等方的な(s 波)スピン三重項超伝導も可能である[1,2]。この機構は以下のように理解することができる。すなわち、異軌道間の電子スピンの間にはフント結合というクーロン相互作用に由来する強磁性的な結合があり、これは同じスピン間の有効引力として働く。しかし、現実の物質ではこのような超伝導が多く実

現しているわけではないため、上記の超伝導がどのような状況下で実現するかを明らかにする必要がある。そこで我々は多軌道ハバードモデルを動的平均場理論によって解析し、スピン三重項超伝導が実現するパラメータ領域を調べた[3]。その結果、この超伝導は Spin-freezing 現象[4,5]という、多軌道電子系特有の物理と関係していることを明らかにした。

さらに、超伝導相は磁気秩序相と隣接しており、かつ転移温度はドーム形状を持つため、相図は一般によく知られている非従来型超伝導体のそれと酷似している。通常、磁気的量子臨界点まわりから生じる非局所的な揺らぎ（マグノン）によるクーパー対形成が考えられているが、本研究で見出された超伝導は Spin-freezing 現象に伴う局所的な磁気揺らぎが重要であり、量子臨界点とは直接の関係がない。セミナーではこの超伝導の機構について詳しく紹介し、現実物質との関連についても議論したい。

この研究は Philipp Werner 氏（スイス Fribourg 大）との共同研究である。

[1] A. Klejnberg and J. Spalek, J. Phys.: Condens. Matter **11**, 6553 (1999).
[2] M. Zegrodnik, J. Bunemann and J. Spalek, New J. Phys. **16**, 033001 (2014).
[3] S. Hoshino and P. Werner, Phys. Rev. Lett. **115**, 247001 (2015).
[4] P. Werner, E. Gull, M. Troyer, and A. J. Millis, Phys. Rev. Lett. **101**, 166405 (2008).
[5] A. Georges, L. d. Medici, and J. Mravlje, Annu. Rev. Condens. Matter Phys. **4**, 137 (2013).