International Workshop

Research Frontier of Advanced Spectroscopies for Correlated Electron Systems

June 13 (Thu) – 15 (Sat), 2019

Institute for Materials Research (IMR), Tohoku University,
Sendai, Japan

Abstract
Venue

Auditorium in the 2nd building of Institute for Materials Research, Tohoku University, Sendai, Japan

Access

Institute for Materials Research, Tohoku University 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan

Access from Sendai Station

- Taxi (10 min) a Taxi Stand at Sendai Station West Exit -> IMR (*KINKEN* in Japanese)
- Subway (8 min) Subway Tozai line for Yagiyama Zoological Park Station [T01] -> Aobadori-Ichibancho Station [T04], South Exit 1 -> Walk
- walk (20 min) West Exit at Sendai Station -> Walk to IMR

Campus Map

Here!
Research Frontier of Advanced Spectroscopies for Correlated Electron Systems

June 13 Thu. – 15 Sat. 2019
Institute for Materials Research (IMR), Tohoku University, Sendai, Japan

June 13 Thursday
13:00 - 13:25 Registration
13:25 - 13:30 Opening, Masaki Fujita (Tohoku Univ.)

Toward High-$T_c$ and Methods
Chairman: M. Fujita (Tohoku Univ.)
13:30 - 13:55 Shin-Ichi Uchida (Chinese Academy of Sciences)
High-Temperature Superconductivity in a Copper Oxide without CuO$_2$ Plane
13:55 - 14:20 Jose Lorenzana (Sapienza Univ.)
Strong Supercexchange from Raman and Neutron Scattering in the Silver Analogue of Cuprates
14:20 - 14:40 Kazuhiko Kuroki (Osaka Univ.)
Possibility of Unconventional High-$T_c$ Superconductivity in Systems with Coexisting Wide and Narrow Bands
14:40 - 15:00 Ryotaro Arita (Univ. of Tokyo)
Self-Energy Variational Approach to Correlated Electron Systems

15:00 - 15:20 Break

Functional Materials
Chairman: K. Kuroki (Osaka Univ.)
15:20 - 15:45 Giniyat Khaliullin (MPI-FKF)
RIXS in 4d-Electron Systems: Probing Magnons, Spin-Orbit Excitations, and Hund’s Multiplets in Ruthenates
15:45 - 16:05 Giacomo Prando (Univ. of Pavia)
Tuning the Magnetocrystalline Anisotropy in RCoPO by Means of R Substitution: A Ferromagnetic Resonance Study
16:05 - 16:25 Michiyasu Mori (Japan Atomic Energy Agency)
Electronic States of Phonon Hall Materials
16:25 - 16:30 Hidetoshi Fukuyama (Tokyo Univ. of Science)
Introduction to the Sir Martin Wood Prize
16:30 - 16:55 Yoshihiko Okamoto (Nagoya Univ.)
Exploration of Novel Transition Metal Compounds Based on the Unique Crystal and Electronic Structures

Posters
16:55 - 17:00 Hiroyuki Yamase (NIMS)
Preview of 11 Posters
17:00 - 18:00 Poster Presentation with Refreshment
List of Posters

Theory
P1. Masahiko Hayashi (Akita Univ.)
   Gaussian-Fluctuation Corrections to the Phase Diagram of t-J Model
P2. Hisatoshi Yokoyama (Tohoku Univ.)
   Filling-Control-Type Mott Transitions in Half-Filled and Partially Filled Impurity Hubbard Models
P3. Muhammad Zafur (Hokkaido Univ.)
   Self-Restraint Effect of Superconductivity due to Spin Fluctuations

T'-Type Cuprates
P4. Shun Asano (Tohoku Univ.)
   Effect of Reduction Annealing on the Electronic States in T'-Type Cuprates Investigated by Cu K-Edge X-Ray Absorption Spectroscopy
P5. Makoto Mitarashi (Tohoku Univ.)
   Single Crystal X-Ray Structure Analysis of T'-Type Cuprate Superconductor via Reduction Annealing

Nickelates
P6. Kenji Ishii (QST)
   Charge Excitations in Hole-Doped Nickelates Probed with Resonant Inelastic X-Ray Scattering at the Oxygen K-Edge

Organic SC
P7. Shiori Sugiura (NIMS)
   Anomalous Energy Dissipation due to Josephson Vortex dynamics in Layered Organic Superconductor

FFLO in CeCoIn$_5$
P8. Takanori Taniguchi (Tohoku Univ.)
   NMR Searching for the FFLO State of CeCoIn$_5$ in a Parallel Field

Fe-SC
P9. Jan Fikacek (Czech Academy of Sciences)
   X-Ray Absorption Spectroscopy Measurements of Fe$_{1+x}$Te
P10. Giacomo Prando (Univ. of Pavia)
   Charge Order and Orbital-Selective Behaviour in Iron-Based Superconductors: What Do Nuclei and Muons Tell Us?

Pyrochlore
P11. Giacomo Prando (Univ. of Pavia)
   Influence of Hydrostatic Pressure and of Eu/Bi Substitution on the Magnetic Properties of Eu$_2$Ir$_2$O$_7$
June 14 Friday

Cuprates I

Chairman: T. Adachi (Sophia Univ.)

9:00 - 9:20 Hideto Fukazawa (Chiba Univ.)

Suppression of Antiferromagnetic Spin Fluctuations by Electron Doping in \( T'\text{-Pr}_{1.3}\text{La}_{0.7}\text{Ce}_x\text{CuO}_4 \)

Probed by NMR

9:20 - 9:40 Takayuki Kawamata (Tohoku Univ.)

Electron Doping in the Undoped (Ce-Free) Superconductor \( T'\text{-La}_{1.8}\text{Eu}_{0.2}\text{CuO}_4 \)

10:05 - 10:30 Andreas Suter (PSI)

Superconductivity Drives Magnetism in \( \delta\)-Doped \( \text{La}_2\text{CuO}_4 \)

10:30 - 10:50 Break

Cuprates II

Chairman: A. Fujimori (Univ. of Tokyo)

10:50 - 11:15 Matthieu Le Tacon (KIT)

Uniaxial Pressure Control of Competing Orders in the Cuprates

11:15 - 11:40 Wei-Sheng Lee (SLAC)

Probing CDW Phenomena and Charge Excitations in Cuprates via RIXS

11:40 - 12:05 Matias Bejas (UNR-CONICET)

Dual Structure in the Charge Excitation Spectrum of Electron-Doped Cuprates

12:05 - 12:25 Masafumi Horio (Univ. of Zurich)

Three-Dimensional Fermi Surface of Overdoped La-Based Cuprates

12:25 - 14:00 Lunch

Cuprates III + Fe-SC I

Chairman: M. Ogata (Univ. of Tokyo)

14:00 - 14:20 Anna Kauch (TU Wien)

\( \pi \)-Fgons - Generic Optical Excitations of Correlated Systems

14:20 - 14:40 Kazuhiro Kuboki (Kobe Univ.)

Spontaneous Magnetic Field near a Time-Reversal Symmetry Broken Surface State of YBCO

14:40 - 15:00 Atsushi Fujimori (Univ. of Tokyo)

ARPES Studies of Electronic Nematic Phases in Cuprate and Iron-Based Superconductors

15:00 - 15:20 Shigeki Miyasaka (Osaka Univ.)

Nematic Fluctuation and Resonance in \( \text{BaFe}_2(\text{As,P})_4 \) Observed by Raman Scattering Spectroscopy

15:20 - 15:40 Seiichiro Onari (Nagoya Univ.)

Quest for the Origin of Various Nematicities in Fe-Based Superconductors

15:40 - 16:00 Break
Fe-SC II
Chairman: S. Tajima (Osaka Univ.)

16:00 - 16:20 Xiang Gang Qiu (Chinese Academy of Sciences)
   *Infrared Spectroscopic Studies of the Phonon Dynamics in Iron-Based Superconductors*

16:20 - 16:40 Weilu Zhang (Sophia Univ.)
   *High-Tc superconductivity in Absence of Nematic Fluctuations in CaKFe$_4$As$_4)*

16:40 - 17:00 Takasada Shibauchi (Univ. of Tokyo)
   *Time-Reversal Symmetry Breaking in the Nematic Superconductor FeSe*

17:00 - 17:20 Tadashi Machida (RIKEN)
   *Nature of Zero-Energy Vortex Bound State in Superconducting Topological Surface State of Fe(Se,Te)*

17:20 - 17:45 Chandan Setty (Univ. of Florida)
   *Topological Ultranodal Pair States in Iron Based Superconductors*

**Discussion + Banquet**

17:45 - 20:00 Discussion + Banquet
June 15 Saturday

Fe-SC III  
Chairman: A. Maeda (Univ. of Tokyo)

9:00 - 9:25 Xing Jiang Zhou (Chinese Academy of Sciences)  
*Insulating Parent Phase and Distinct Doping Evolution to Superconductivity in Single-Layer FeSe/SrTiO₃ Films*

9:25 - 9:45 Kosuke Nakayama (Tohoku Univ.)  
*Superconductivity and Fermiology in Atomically-Thin Iron-Chalcogenide Films Studied by ARPES*

9:45 - 10:05 Fuyuki Nabeshima (Univ. of Tokyo)  
*Comparison between Te- and S-Substitution Effects on Superconductivity in FeSe Thin Films*

10:05 - 10:25 Takahiro Shimojima (RIKEN)  
*Ultrafast Nematic-Orbital Excitation in FeSe*

10:25 - 10:45 Break

Interesting Systems I  
Chairman: T. Tohyama (Tokyo Univ. of Science)

10:45 - 11:05 Yusuke Nambu (Tohoku Univ.)  
*Dynamical Magnetism in Iron-Based Ladder Compounds*

11:05 - 11:25 Kazutaka Kudo (Okayama Univ.)  
*Exploration of Novel Pt-Based Superconductors with Honeycomb Networks*

11:25 - 11:45 Shingo Yonezawa (Kyoto Univ.)  
*Observation and Control of Nematic Superconductivity in Doped Bi₂Se₃ Topological Superconductors*

11:45 - 12:05 Tsutomu Nojima (Tohoku Univ.)  
*Effect of Antisymmetric Spin-Orbit Interaction on Critical Field of Ion-Gated 2D Superconductors*

12:05 - 12:25 Shinya Uji (NIMS)  
*Fulde-Ferrell-Larkin-Ovchinnikov Phases in Layered Organic Superconductors*

12:25 - 13:40 Lunch

Interesting Systems II  
Chairman: H. Kontani (Nagoya Univ.)

13:40 - 14:00 Marie-Aude Méasson (CNRS- Néel Institute)  
*Collective Mode of the Hidden Order State in URu₂Si₂: Degeneracy and Symmetry*

14:00 - 14:20 Kenji Ishida (Kyoto Univ.)  
*NMR Studies on U-Based Ferromagnetic Superconductors*

14:20 - 14:40 Akito Daido (Kyoto Univ.)  
*Nonsymmorphic Topological Superconductivity in the Paramagnetic Superconducting Phase of UCoGe*

Summary + Discussion

14:40 - 15:00 Hiroyuki Yamase (NIMS)  
*Summary of the Workshop*

15:00 - 17:00 Discussion
June 13 (Thu)

Oral Presentation
High-temperature superconductivity in a copper oxide without CuO$_2$ plane

S. Uchida

Department of Physics, University of Tokyo, Japan
Institute of Physics, Chinese Academy of Sciences, Beijing, China

A great many families of layered copper oxides (cuprates) have been found to show high-$T_c$ superconductivity with a CuO$_2$ plane as the common structural ingredient. One of the fundamental questions for understanding high-$T_c$ superconductivity is: what are the optimal conditions for highest $T_c$. Although a clear answer to this question has not been given yet, consensus hypotheses include: 1) perfect CuO$_2$ plane, 2) a low or moderate density of doped holes (electrons) in the CuO$_2$ planes, and 3) the out-of-plane apical oxygen atoms being well distant from the neighboring plane. The present work reports the discovery of a new high-$T_c$ cuprate with the simple chemical formula Ba$_2$CuO$_{4-y}$ which is synthesized under high pressure. In the new superconductor high-$T_c$ superconductivity occurs in highly oxygen deficient Cu-O planes with heavily overdoped holes and with the apical-O located very close to the plane, evidenced by neutron diffraction and Cu L$_3$-edge and O K-edge XAS. These contradict all of these currently accepted hypotheses. Intriguingly, this new cuprate contains a large amount of oxygen vacancies in the plane, signaling a new Cu-O structure - different than the previously known CuO$_2$ plane - that also sustains high-$T_c$ superconductivity.

The present work has been performed in collaboration with C.Q Jin, W.M. Li, L.P. Cao, J.F. Zhao, Y. Liu, Q.Q. Liu, (IOP, Beijing), Z. Hu (MPI, Dresden), Q.Z. Huang, H. Wu (NIST, Gaithersburg), H.J. Lin, C.T. Chen (NSRRC, Hsinchu), Z. Li (Nanjing University of Science and Technology), Z.Z. Gong, Z. Guguchia, Y.J. Uemura (Columbia University), J.S. Kim, G. Stewart (University of Florida).
Strong Superexchange from Raman and Neutron Scattering in the Silver Analogue of Cuprates

J. Gawraczyński,1 D. Kurzydłowski,2 R. A. Ewings,3 S. Bandaru,1 W. Gadomski,4 Z. Mazej,5 G. Ruani,6 I. Bergenti,6 K. Tokár,7 M. Derzsi,8 P. Barone,9 J. Lorenzana,10 W. Grochala1

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3 ISIS Facility, Rutherford Appleton Laboratory, United Kingdom
4 Faculty of Chemistry, University of Warsaw, Poland
5 Jožef Stefan Institute, Ljubljana, Slovenia
6 ISMN, CNR, Bologna, Italy
7 Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia
8 Advanced Technologies Research Institute, STU, Trnava, Slovakia
9 SPIN, CNR, Chieti, Italy
10 ISC and Sapienza University, CNR Rome, Italy

Analogs of cuprates without copper can pave the way to new quantum materials exhibiting exotic magnetic states and perhaps new high-Tc superconductors. Despite several attempts, materials that reproduce the key cuprate characteristics (spin-1/2, quasi-two-dimensional behavior, and high superexchange constant) have not been found. A natural choice is to replace Cu d9 by Ag d9. As will be discussed, this requires replacing O by F to retain a positive charge transfer energy. AgF2 (Fig. 1) results to be an excellent analog of parent cuprates. Density functional theory show remarkably similar electronic parameters in both materials. Furthermore, Raman and Neutron scattering show that the superexchange interaction reaches 70% of cuprates[1]. We argue that structures that reduce or eliminate the buckling of the AgF2 planes could have an antiferromagnetic coupling that matches or surpasses the cuprates potentially leading to high-Tc superconductivity.

Figure 1: Schematic view of an AgF2 plane.

Possibility of Unconventional High-\(T_c\) Superconductivity in Systems with Coexisting Wide and Narrow Bands

Kazuhiko Kuroki
Department of Physics, Osaka University, Toyonaka, Osaka, 560-0043 Japan

One possible scenario for high-\(T_c\) superconductivity is to have strong pairing interaction and light electron mass at the same time, but strong pairing interaction usually induces heavy effective mass. In ref.[1], the present author proposed that high-\(T_c\) superconductivity is possible in repulsively interacting systems having wide and narrow bands, where light effective mass and strong pairing interaction is realized when the Fermi level sits near the narrow band edge. The two-leg Hubbard ladder with diagonal hoppings, a model for the ladder-type cuprates, was studied as a system in which such a situation is realized, where a possible occurrence of extremely high \(T_c\) was suggested if a large amount of electrons can be doped.

In the former part of the present talk, we extend this study and show that this high-\(T_c\) mechanism works in a variety of systems that consist of wide and narrow (or flat) bands, such as the diamond lattice and the three-leg ladder in one dimension, and the bilayer (square, triangular, or honeycomb) lattices in two dimensions. We apply the fluctuation exchange approximation to the Hubbard model on these lattices, and show that superconductivity is strongly enhanced when the Fermi level sits close to the narrow band edge [2]. This shows the generality of the mechanism of high-\(T_c\) superconductivity originating from wide and incipient narrow bands. In the latter part of the talk, we propose possible ways to realize situations favorable for superconductivity in actual materials. First, we consider ladder-type cuprates, where lattice deformation is introduced. We show how the lattice deformation affects the electronic band structure, and hence superconductivity. Secondly, we introduce a concept of “hidden ladder” electronic structure in the bilayer Ruddlesden-Popper compounds, where anisotropic \(d\)-orbitals give rise to ladder-like electronic structures [3]. Namely, considering the case in which \(t_{2g}\) orbitals form the bands crossing (or lie near) the Fermi level, an electron in the \(d_{xz/yz}\) orbital selectively hops in the \(x/y\) direction as well as in the \(z\) direction normal to the bilayer. This means that the \(d_{xz/yz}\) orbitals form ladders with \(x/y\) and \(z\) directions being the leg and rung directions, respectively. We propose that \(\text{Sr}_3\text{Mo}_2\text{O}_7\) and \(\text{Sr}_3\text{Cr}_2\text{O}_7\) are candidates for the hidden ladder materials where the Fermi level sits in the vicinity of the narrow-band edge without large amount of carrier doping.

References:
Self-energy variational approach to correlated electron systems

Shiro Sakai¹, Ryotaro Arita¹,²

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In the Kohn-Sham theory, we map the full interacting system with the real potential, onto a fictitious non-interacting system whereby the electrons move within an effective single-particle potential. We then solve the so-called Kohn-Sham equation self-consistently, and obtain the spectral function. This approach works very successfully for weak correlated electron systems, and has been applied to a variety of materials. However, it has been well known that the Kohn-Sham energy cannot represent the spectral function of strongly correlated electron systems. For example, we have no chance to reproduce the Mott-Hubbard gap in a Mott insulator.

In this talk, we propose a new nonperturbative numerical method, which we call self-energy variational approach, to study correlation problems in solids. The method is based on a discretized spectral representation of the electron self-energy, which can be interpreted as a hybridization of electron with auxiliary fermionic degrees of freedom. Our approach has many advantages over the Kohn-Sham approach or existing many-body approaches: It is efficient and numerically inexpensive, since we just solve an effective one-body problem. It can be applied to systems with any dimension, any dispersion, and any two-particle interaction. Taking the two-dimensional Hubbard model as a representative example, we show how the method works successfully (Fig.1).

Figure 1: Spectral function of the two-dimensional Hubbard Model. We compare the results obtained by the present method (left) and Quantum Monte Carlo calculation for finite systems (right, taken from Moukouri and Jarrell, PRL 87, 167010 (2001)), where we see a good agreement.
RIXS in 4d-electron systems: Probing magnons, spin-orbit excitations, and Hund’s multiplets in ruthenates

Giniyat Khaliullin
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Ruthenium compounds serve as a platform for unconventional magnetism and superconductivity. In ruthenates, several key parameters such as spin-orbit coupling, Hund’s interaction, crystal-field splittings, and exchange interactions are comparable in magnitude, and their interplay is essential for understanding the physical properties of these compounds. We will present the recent Ru L-edge resonant inelastic x-ray scattering (RIXS) data [1,2] on ruthenium oxides SrRu$_2$O$_6$ and Ca$_2$RuO$_4$, and show how the above interaction parameters can be extracted from the RIXS data using a simple model calculations. In quasi-two-dimensional SrRu$_2$O$_6$, we observe a large magnon gap which is driven by spin-orbit coupling and chiefly responsible for unusually high Néel temperature (560 K) of this material. In Ca$_2$RuO$_4$, we observe composite spin-orbit excitations and Hund’s-rule driven spin-state transitions. The parameters inferred from the RIXS data are consistent with the previous INS results [3] and strongly support the picture of excitonic magnetism [4] in Ca$_2$RuO$_4$.

* This work was supported by the European Research Council under Advanced Grant No. 669550 (Com4Com).
2) H. Gretarsson et al., unpublished.
Tuning the magnetocrystalline anisotropy in RCoPO by means of R substitution: a ferromagnetic resonance study

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¹Department of Physics, University of Pavia, Pavia, Italy
²Leibniz-IFW Dresden, Dresden, Germany
³National Physical Laboratory, New Delhi, India

In RCoPO oxides, both the transition temperature to the itinerant ferromagnetic phase $T_C$ and the volume of the crystallographic unit cell $V$ are conveniently tuned by the $R$ ionic radius and/or by external pressure. In particular, we have demonstrated [1,2] a linear correlation between $T_C$ and $V$ by means of muon-spin spectroscopy measurements under hydrostatic pressure and ab initio calculations, demonstrating a full equivalence of chemical and external pressures on a quantitative level. The experimental evidences suggest that $R$ ions influence the ferromagnetic phase only via the induced structural shrinkage without involving any active role from the electronic $f$ degrees of freedom. These latter are only giving a sizable magnetic contribution at much lower temperatures.

Here, we report on broad-band electron-spin resonance measurements performed within the itinerant ferromagnetic phase of RCoPO ($R =$ La, Pr, Nd, and Sm) [3]. We reveal that the $R$ substitution is highly effective in gradually introducing a sizable easy-plane magnetocrystalline anisotropy within the Co sublattice (see figure). We explain our results in terms of a subtle interplay of structural effects and of indirect interactions between the $f$ and $d$ orbitals from $R$ and Co, respectively. Our observations provide interesting information on the crucial role of $R$ ions in affecting the electronic properties of the CoP layers, of possible interest also for the isostructural FeAs-based family of high-$T_c$ superconductors.

Figure: Experimental ferromagnetic resonance lines at comparable frequencies for the four investigated samples at different temperature values safely within the FM phase. The vertical dashed line denotes the central position for the resonance line of LaCoPO. Curves are shifted vertically for the aim of clarity.

Electronic states of phonon Hall materials

Michiyasu Mori

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The phonon Hall effect (PHE) on a heat current is an analogue of the Hall effect on a charge current. The heat current carried by phonons induces a transverse temperature drop in a magnetic field. The phenomenon was observed in the paramagnetic insulator, Tb$_3$Ga$_5$O$_{12}$ (TbGG) [1,2,3]. Since the TbGG has a large band gap of several eV, only phonons can carry the heat at low temperatures. Another non-magnetic insulator, Ba$_3$CuSb$_2$O$_9$ (BCSO), also shows the PHE [4]. The BCSO is in the spin liquid state with the spin gap of about 50 K [5]. The heat transport at lower than 50 K must be dominated by phonons instead of spinons. In both cases, phonons do not have charge nor spin, so that an origin of the PHE is an interesting problem.

In the former half, we will discuss a resonant scattering of phonons at a Tb$^{3+}$ ion, which induces the skewness of phonon current in the TbGG [6]. The resonances are given by the crystal field (CF) levels of a Tb$^{3+}$ ion, which has a large total angular momentum $J=6$. When the CF potential is expanded with respect to lattice strains, the first term is a coupling between a quadruple and a strain due to $J=6$. This plays a role of spin-phonon coupling. Some magnetic-field dependences of CF levels will be discussed by considering inelastic neutron scattering data.

In the latter half, we will discuss the BCSO, that does not contain any ion with large $J$ such as Tb$^{3+}$ ion. It is composed of only spin-1/2 isotropic in the charge degree of freedom. Hence, we need to find a coupling between spin and phonon. One possibility is a spin-phonon coupling. Some magnetic-field dependences of CF levels will be discussed by considering inelastic neutron scattering data.

In the latter half, we will discuss the BCSO, that does not contain any ion with large $J$ such as Tb$^{3+}$ ion. It is composed of only spin-1/2 isotropic in the charge degree of freedom. Hence, we need to find a coupling between spin and phonon. One possibility is an orphan spin, which is an additional Cu$^{2+}$ spin located in the center of Cu$^{2+}$ hexagonal. It is said that the BCSO contains about 5%~16% of the Cu$^{2+}$ orphan spins and its thermal conductivity in low temperatures is dominated by scattering at orphan spins [4]. We will discuss a mechanism that a hexagonal cluster centered on an orphan spin makes a spin-phonon coupling and leads to the PHE.

* This work is done in collaboration with A. Spencer-Smith, O. P. Sushkov, S. Maekawa, H. Kusunose, M. Fujita, Y. Nambu, S. Kawamura, M. Kofu, and K. Nakajima, and is supported by MEXT KAKENHI JP16H01082 and JP18H04492.

Exploration of Novel Transition Metal Compounds Based on the Unique Crystal and Electronic Structures

Yoshihiko Okamoto
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Novel transition metal compounds with remarkable electronic properties, such as cuprate and iron-based superconductors, have opened up a new era of the condensed matter physics. In this talk, I will present the results of materials exploration of transition metal compounds using the crystal and electronic structure databases based on knowledge of solid state chemistry, toward the discovery of such electronic properties and functions. We developed various materials including high-performance thermoelectric materials [1,2], candidate nodal-line semimetals [3,4], superconductors, metal-insulator transition systems, and geometrically frustrated magnets. In this talk, I will focus on the former two systems.

1D telluride Ta₄SiTe₄ as a high-performance thermoelectric material. Thermoelectric cooling is a promising all-solid-state cooling technology, expected to be widely used in local cooling of cryogenic devices. However, there is currently no bulk material with a high enough performance to reach a practical level below −50 °C. We found that Ta₄SiTe₄ and its substituted compounds show high thermoelectric performance at low temperature [1,2]. Thermoelectric power of Ta₄SiTe₄ whisker crystals, shown in Fig. 1, reaches $S = -400 \, \mu V \, K^{-1}$ at 100-200 K, while maintaining low electrical resistivity of $\rho \sim 2 \, m\Omega \, cm$. These $S$ and $\rho$ yield a roughly twice larger power factor ($P = S^2/\rho$) than that in Bi₂Te₃-based practical materials at room temperature. This large value is probably caused by a very small spin-orbit gap opening on strongly one-dimensional electronic bands at the Fermi energy.

CaAgP and CaAgAs as a candidate nodal-line semimetal. In recent years, Dirac and Weyl semimetals, which are zero-gap semiconductors with linear dispersion bands at the zero-gap points, have attracted broad interest as candidate systems for realizing topologically nontrivial states in bulk materials. In contrast, some systems are theoretically indicated to have a nodal line, where the linear dispersion bands cross on a line in the momentum space. We found that CaAgP and CaAgAs are promising candidates for the nodal-line semimetal. First principles calculation results indicate that the both compounds are ideal nodal-line semimetals, where the Dirac points form a ring at the Fermi energy [3]. We synthesized polycrystalline samples and single crystals of CaAgP and CaAgAs (Fig. 2) and experimentally demonstrated that they have a ring-torus Fermi surface related to the nodal ring [4].

June 13 (Thu)

Poster Presentation
Gaussian-fluctuation Corrections to the phase diagram of \( t-J \) model

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The \( t-J \) model in the slave-boson approach is one of the promising model to describe high-Tc superconductivity in cuprates. In this paper, we study the fluctuation effects on the phase diagram of the \( t-J \) model by self-consistently incorporating the Gaussian fluctuations around the equilibrium values of the order parameters. We especially pay attention to the superconducting (SC) and the antiferromagnetic (AF) order. Since the nonlinearity of the free energy functional of the \( t-J \) model is subtle and complicated\(^1\), we do not use the so-called Ginzburg-Landau type expansion. Instead, we use the self-consistent harmonic approximation, which enables us to treat the nonlinearity in a non-perturbative way. In the figure, the mean-field (MF) results and the fluctuation corrected ones using the present method (SCHA) are shown: (a) is the behavior of the AF and SC order parameters as a function of the temperature, and (b) is the phase diagram of the \( t-J \) model. Significant suppression of the orders by the effects of fluctuation can be seen. Although our method is not very useful near the critical points, we believe it gives overall picture of the fluctuation effects in \( t-J \) model with a desirable accuracy. We studied only the thermal (classical) fluctuations here, however the present method can also treat quantum ones.

\( \delta = 0.1428 \)

Figure 1: (a) Temperature \( T \) dependence of the AF and SC order parameters in the \( t-J \) model. Here, \( \delta \) is the doping. (b) The fluctuation-corrected phase diagram of the \( t-J \) model. In each figure, MF and SCHA indicates the results of mean-field and self-consistent harmonic approximation. In (a), the transition temperatures of AF and SC are reversed due to the inclusion of the fluctuation effects.

\[ * \] This work was supported by JSPS KAKENHI Grant Numbers 24540392 and 15K04619.

Filling-Control-Type Mott Transitions in Half-Filled and Partially Filled Impurity Hubbard Models

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² Department of Natural Science, Chiba Institute of Technology, Narashino 275-0023, Japan
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Cuprates superconductors are doped Mott insulators with inherent impurities as carrier dopants in block layers. Apical oxygen atoms in T* systems typical for electron-doped cuprates also work as impurity sources. In such backgrounds, we have studied the effects of point-type impurity potential in an impurity Hubbard (t-t'-U-V) model on the basis of variational Monte Carlo (VMC) calculations [1-3]. In constructing many-body trial states for the disordered systems, we should be careful in treating the effects of one-body impurity potential V, which intricately competes or concert with local electron correlations. Recently, we found that the addition of a one-body projection factor P(θ) for V [4] is effective for the convergence in the VMC optimization [2,3]. Thereby, we became able to carry out systematic calculations for arbitrary V.

In this presentation, we would like to summarize recent results regarding impurity-induced Mott transitions obtained using P(θ) for an antiferromagnetic state, which is more insulative than a paramagnetic [2] or a d-wave superconducting states [3]. (i) At half filling: The state is always insulating for U > 0 in the uniform case. When |V| is increased in the Mott regime (U > band width), however, the state becomes metallic at V = V_U^(±), with |V_U| ~ U - |E_c|. Here, E_c (~ t) is the kinetic energy of the carriers for V > V_U^(±) (electrons or doublons) or V < V_U^(-) (holes or holons). In this filling, the behavior for attractive (V < 0) and repulsive (V > 0) potentials is connected through a canonical transformation. (ii) In partially filled cases: For V < 0, the state is always metallic, continued to the uniform case (V = 0), where the state is always metallic. For V > 0, the behavior is different according to the relation between the doping rate δ and the impurity-site density δ_imp. (a) For δ_imp < δ, the state is always metallic. (b) For δ_imp = δ, the state becomes insulating for V > V_M (~ t). (c) For δ_imp > δ, the state becomes insulating for V_M < V < V_U^(±). We can intuitively interpret such behavior by virtue of Mott physics. We also would like to refer to large-δ_imp cases.

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Self-Restraint Effect of Superconductivity due to Spin Fluctuations

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It is well known that antiferromagnetic spin fluctuations can drive superconductivity. In particular, this scenario is widely discussed for iron-based superconductors [1,2]. However, a recent theoretical study in a minimal two-band model of iron-based superconductors [3] shows that aside from the tendency to drive superconductivity, spin fluctuations also have a contribution to suppress the superconducting instability itself. This “self-restraint effect” comes from scattering processes inside the same Fermi pocket with small momentum transfer, which corresponds to a “tail” of spin fluctuations. It is interesting that such a seemingly negligible contribution plays a remarkably important role in the superconducting mechanism. Therefore, in this work, we explore the generality of the self-restraint effect to fully understand the role of spin fluctuations in superconductivity by employing a one-band model with a typical Fermi surface of cuprate superconductors.

Effect of reduction annealing on the electronic states in T'-type cuprates investigated by Cu K-edge X-ray absorption spectroscopy

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For the emergence of superconductivity in T'-type $RE_2_xCe_xCuO_4$ ($RE =$ rare earth element), a post-annealing procedure in a reducing atmosphere as well as the electron-doping by Ce substitution is necessary. Therefore, the variation of electronic states due to annealing is important to understand the microscopic mechanisms of anneal-induced superconductivity. Recent studies of photoemission spectroscopy and soft x-ray absorption spectroscopy suggest an electron-doping by oxygen non-stoichiometry brought through the annealing \cite{1-3}. However, the relationship between the oxygen contents and the electron number have not yet been clarified quantitatively.

We, therefore, investigate the Ce substitution and reduction annealing effects on the electronic states at the Cu sites using Cu K-edge X-ray absorption spectroscopy measurements with transmission mode \cite{4}. The evolution of the electronic states against oxygens variation ($\delta$) at several $x$ values in Pr$_{2-x}$Ce$_x$CuO$_{4+\delta}$ (PCCO) was measured systematically using polycrystalline samples. The variation in the absorption spectra induced by the annealing are qualitatively similar to the case of Ce substitution in entire $x$, indicating an aspect of electron doping in the annealing effect. Moreover, we evaluate the relative electron number by the integrate intensity of 1s-4p$\pi$ dipole transition for Cu$^\ast$. From the analysis, the electron number by Ce substitution $n_{Ce}$ increases linearly with $x$ in as-sintered PCCO, whereas the number of additionally introduced electrons by annealing $n_{AN}$ does not follow a simple relation $n_{AN} = 2\delta$, which is excepted from charge neutrality. The larger value of $n_{AN}$ than $2\delta$ suggests the emergence of not only electrons but also holes due to annealing.

Single crystal X-ray structure analysis of T'-type cuprate superconductor via reduction annealing

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The electron-doped cuprates with the T'-structure require oxygen reduction annealing to induce superconductivity. In recent years, unlike conventional reduction in inert gas, induction of superconductivity in the non-doped regime has been confirmed for thin film samples by reduction annealing in a low oxygen partial pressure environment [1]. Inspired by that study, single crystals induce super superconductivity in the under-doped regime by using polycrystalline powders which have the same composition (protect annealing method) [2]. From the above, it is important to elucidate the structural change via annealing process. The following two points are described regarding structural change. One is that there is excess oxygen called apical oxygen at the top and/or bottom of CuO$_2$ plane and CuO$_2$ plane is optimized for superconductivity by removing apical oxygen [3]. The other is that secondary phase RE$_2$O$_3$ with different structure from the parent phase is precipitated by reduction [4], which compensates for a few percent of Cu defects observed in the as-grown state and CuO$_2$ plane is optimized for superconductivity [5].

In this study, we performed single crystal X-ray structure analysis about Pr$_{2-x}$La$_x$CuO$_{4+\delta}$, Nd$_x$CuO$_{4+\delta}$ and Pr$_{1.3-x}$La$_{0.7}$Ce$_x$CuO$_{4+\delta}$ ($x = 0.10$) (PLCCO) and were able to analyze them with high accuracy of reliability factor 1.5%. Cu defects was confirmed in all as-grown samples and compensated in all reduced samples with appearance of the secondary phase.

None of as-grown, protect annealing (protect reduced) and protect annealing + low temperature annealing + dynamic annealing (dynamic reduced) samples of PLCCO indicate oxygen deficiency in the parent phase (Table 1). On the other hand, volume fraction of the secondary phase increases as reduction condition becomes stronger from the comparison of normalized Bragg peak intensities of the secondary phase (Figure 1). Therefore, it is considered that oxygen deficiency due to reduction is used for the secondary phase RE$_2$O$_3$ formation and the parent phase is electron-doped (Table 1 Cu bond valence).

| Table 1: O occupancy and Cu valence of each sample |
|----------------|----------------|----------------|
|                | PLCCO as-grown | protect reduced |
| O1 acc. (%)    | 101.7(7)       | 102.3(5)        |
| O2 acc. (%)    | 103.1(6)       | 102.4(5)        |
| Cu bond valence| 1.728(5)       | 1.7245(5)       |

Charge excitations in hole-doped nickelates probed with resonant inelastic x-ray scattering at the oxygen K-edge

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Effect of carrier doping into insulating transition-metal oxides is a central issue in correlated electron systems and parent insulators are categorized into two types: Mott insulators and charge-transfer insulators [1]. In the latter, the energy of charge transfer (Δ) from the oxygen 2p to the transition-metal d levels is smaller than the on-site Coulomb repulsion (U) of the d electrons. When holes are doped into the charge-transfer insulators, they predominantly occupy the oxygen 2p orbitals. This is the case for the high-Tc superconducting cuprate La2-xSrxCuO4 as well as its isostructural nickelate La2-xSr2NiO4.

Existence of the oxygen 2p holes has been confirmed by x-ray absorption spectroscopy (XAS) at the oxygen K-edge [2,3]. Then, the experimental technique is naturally extended to resonant inelastic x-ray scattering (RIXS) for measuring charge excitations of doped holes. Since single spin-flip excitations are forbidden, charge excitations are mainly observed by the oxygen K-edge RIXS. In fact, we recently succeeded to observe charge excitations in hole-doped cuprates and clarified that magnitude of momentum dependence of the charge excitations is on the order of eV [4].

As a comparative study of the cuprates, we present oxygen K-edge RIXS on the hole-doped nickelates La2-xSr2NiO4+δ with hole density (nh = x + δ) of 0.10 and 0.33. The RIXS experiment was performed using the HORNET spectrometer at BL07LSU of SPring-8. Tuning the incident photon energy to the hole peak in XAS, Raman-like spectral weight is observed below 2 eV. Because the spectral weight is located below the charge-transfer gap of the parent La2NiO4 (∼4 eV) and well-above the magnetic excitations, it is ascribed to the charge excitations of the doped holes. In stark contrast to the cuprates, the momentum dependence of the charge excitations is found to be very weak in the nickelates, indicating that the doped holes are localized in the NiO2 plane. The localized character of holes is consistent with the insulating behavior in conductivity [5] and it could be an origin of wider hole density of charge-stripe ordered phase in the nickelates than that in the cuprates [6].

Anomalous Energy Dissipation due to Josephson Vortex dynamics in Layered Organic Superconductor

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Layered superconductors have attracted much interest because of their fascinating properties in magnetic fields. One of the most intriguing features is a peak effect in the field/temperature dependence of interlayer resistance near $H_{c2}/T_c$.[1] The behavior, which has been found in high $T_c$ cuprates and layered organic superconductors, is regarded as a universal feature in highly two-dimensional superconductors. Although some theoretical models have been proposed to explain it, no satisfactory explanation has been given.

To further investigate the origin of the peak, we have performed systematic measurements of the interlayer resistance in a highly two-dimensional organic superconductor $\beta''$-(ET)$_2$SF$_5$CH$_2$CF$_2$SO$_3$ salt. Figure 1 presents the interlayer resistance in magnetic fields perpendicular to the layers at various currents. For a high-quality sample (#1), a peak at ~1.2 T below $H_{c2}$ (~1.8 T) is enhanced with increasing current, whose resistance is apparently higher than the normal state value. For a low-quality sample (#2), the interlayer resistance monotonically increases with increasing field (no peak behavior is seen).

It is known that characteristic magnetic flux line structures in superconducting states appear in layered superconductors, which are composed of pancake and Josephson vortices.[2,3] Even in perpendicular fields, Josephson vortices can be thermally excited between the layers. Such Josephson vortices will be strongly driven by the perpendicular current. If the pinning force is sufficiently small, large energy dissipation due to driven vortices could happen.[2] The peak resistance larger than the normal state value in Fig. 1(a) suggests that vortices are driven at an anomalously high velocity. We will also present the results at various temperatures and field angles.

Figure 1: Magnetic field dependences of the interlayer resistance of (a) high-quality (#1) and (b) low-quality (#2) samples at 0.6 K for various current values, respectively. Insets show the Shubnikov-de Haas oscillations.

3) S. Sugiura et al., npj Quantum Matter 4, 7, 1 (2019).
NMR Searching for the FFLO state of CeCoIn$_5$ in a parallel field

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The Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state was predicted half a century ago [1, 2], and is one of the exotic superconducting (SC) state. In the heavy fermion superconductor CeCoIn$_5$, it has been reported from various experiments that the FFLO state exists near upper critical field $H_{c2} \sim 5 \pm 1(2)$ T for $H \parallel c (ab)$ as shown in Fig. 1[3]. In addition, various measurements also suggested the field-induced criticality near $H_{c2}$ in $H \parallel c$ and $H \parallel ab$ [3, 4]. Although the novel magnetic state called “Q-phase” was identified in $H \parallel ab$, the magnetic properties near $H_{c2}$ in $H \parallel c$ have not been fully investigated.

The purpose of our research is (1) the investigation of electronic state at the FFLO state, (2) the searching of the field-induced critical point, and (3) revealing the relationship between two phenomena on CeCoIn$_5$ for $H \parallel c$ with NMR and ac susceptibility measurements.

$^{59}$Co-NMR lines split upon entering the superconducting phase and the field dependence of ac susceptibility shows the step-like jump behavior above 4.7 T. Since such behavior were not observed below 4.5 T, these indicate that SC transition becomes the first order, and consistent with the existence of FFLO state reported previously [5, 6].

As for the field-induced criticality, the field dependence of nuclear spin-lattice relaxation rate ($1/T_1$) at 100 mK has a peak at 5.2 T. But, at 5.2 T, the temperature dependence of $1/T_1 T$ increases with decreasing temperature down to 200 mK and saturates below 200 mK, suggesting that the critical point is not located at 0 K but at a finite temperature. Although we observed the development of the AFM fluctuation down to 200 mK, we couldn’t find any trace of magnetic anomaly near $H_{c2}$.

In this presentation, we are planning to present the more details with the temperature dependence of NMR spectra and $1/T_1 T$ near $H_{c2}$.

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X-ray absorption spectroscopy measurements of Fe$_{1+x}$Te

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In our presentation, we show results of X-ray absorption spectroscopy (XAS) measurements of Fe$_{1+x}$Te single crystals with a slight excess of iron ($x < 0.1$).

Iron-based chalcogenides (IBC) are quasi two-dimensional in their crystal structure consisting of Te-Fe-Te trilayers stacked along the c-axis and bound by van der Waals forces. IBC has the simplest crystal structure among iron-based superconductors that predestinates them as ideal candidates for both experimental and theoretical investigations. FeSe was found to be superconducting below a critical temperature of $T_c = 8\, \text{K}$ [1]. The superconducting pairing mechanism is believed to be unconventional, i.e. not phonon-mediated. In recent years, the interest in IBC was further triggered by a discovery that the superconducting transition temperature of FeSe can be enhanced above 100 K when a monolayer of FeSe is grown on SrTiO$_3$ [2, 3]. For an overview, see e.g. [4].

FeTe is the parent compound to FeSe. Contrary to FeSe, bulk FeTe is not superconducting and orders bicollinearly antiferromagnetic below 80 K. Thin films grown on topological insulators have shown indications of superconducting correlations coexisting with this magnetic order [5]. The spin structure and ordering temperature depends on the amount of iron excess. Interestingly, mixed alloys FeTe$_{1-x}$Se$_x$ are superconducting with transition temperatures higher than those of pure FeSe ($T_c = 14.5\, \text{K at } x = 0.5$). Thus, also the understanding of magnetism and electronic properties of FeTe is important as to reveal the origin of superconductivity in IBC. For this, we conducted XAS measurements at the Swiss Light Source in Villigen on Fe-rich Fe$_{1+x}$Te single crystals. Using different photon polarizations, we determined X-ray magnetic circular dichroism (XMCD) and X-ray magnetic linear dichroism (XMLD). XMCD signals scale linearly with the bulk magnetization measured by a SQUID magnetometer and show a characteristic drop when FeTe enters the antiferromagnetic state below $T_N \sim 70\, \text{K}$. In contrary, XMLD signals increase monotonically below $T_N$ down to lowest temperatures $\sim 2\, \text{K}$. XMLD data are compared with results of our density functional theory calculations.

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Charge order and orbital-selective behaviour in iron-based superconductors: what do nuclei and muons tell us?

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A common aspect shared by different classes of iron-based superconductors is the band structure at the Fermi energy, where several bands originating from the 3d orbitals of Fe contribute to the density of states. In the presence of strong electronic correlations, the Hund coupling may promote the occupancy of a single band and decouple the interband charge correlations, yielding to markedly different properties for the electron excitations in the different bands. Significant electronic correlations may also lead to charge-ordered phases which, however, remain experimentally elusive in iron-based superconductors, at variance with the phenomenology observed in cuprate oxides in the underdoped regime.

Here, we report on our investigations [1,2] of the superconductors RbFe\textsubscript{2}As\textsubscript{2} and CsFe\textsubscript{2}As\textsubscript{2}. These materials are close to the condition of half-band filling and are characterized by significant electronic correlations. We observe that the $^{75}$As nuclear quadrupole resonance spectrum progressively broadens upon cooling the sample at temperatures lower than $T_0 \approx 150$ K and 75 K (for RbFe\textsubscript{2}As\textsubscript{2} and CsFe\textsubscript{2}As\textsubscript{2} respectively) and that eventually it splits into two distinct peaks for RbFe\textsubscript{2}As\textsubscript{2} powders. The overall shape in the low-temperature regime is similar to what is expected for incommensurate charge-density wave phases, where the charge ordering modulates the electric field gradient probed by the nuclei. The change in the local charge distribution at $T_0$ also affects the relaxation rate measured by muon spin rotation, likely due to a change in the implantation site of the muon.

The low-energy spin excitations are also studied by measuring, after a proper radio-frequency pulse, the recovery of the $^{75}$As nuclear magnetization pulse towards the equilibrium. Although this phenomenon is described by a single exponential function characterized by the spin-lattice relaxation rate $1/T_1$ at temperatures higher than 20 K, we observe a second and much slower exponential component at lower temperatures for RbFe\textsubscript{2}As\textsubscript{2} powders. We interpret this phenomenology as indication of an orbital-selective condition leading to electronic phase separation. In support of our interpretation, the temperature dependence of $1/T_1$ for the fast-relaxing component is characteristic of a strongly-correlated electron system approaching localization, but the slow-relaxing component shows a temperature dependence of $1/T_1$ which is more characteristic of a weakly-correlated metal.

Influence of hydrostatic pressure and of Eu/Bi substitution on the magnetic properties of Eu$_2$Ir$_2$O$_7$


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The arrangement of magnetic moments at the vertices of a pyrochlore lattice leads to a great variety of electronic ground states for $R_2M_2$O$_7$ materials. One important finding common to several families of these oxides is that changes in $n_I$, the ionic radius of the rare-earth ion $R^{3+}$, gradually tune the local crystalline environment around the transition metal ion $M^{4+}$ and the overall electronic behavior of the compound in turn. For $M = $ Ir, the characteristic temperature $T_{MI}$ for the development of a metal-to-insulator transition is directly controlled by the average value $n_I$ related to a gradual chemical substitution. Moreover, the metal-to-insulator transition in $R_2$Ir$_2$O$_7$ is associated with a dramatic change in the magnetic behavior as well.

Here, we report on the magnetic properties of Eu$_2$Ir$_2$O$_7$ under pressure, both from dc magnetometry and $\mu$SR [1]. The absence of a localized magnetic moment from $f$ shells in Eu$_2$Ir$_2$O$_7$ is a great advantage in the study of the intrinsic magnetic properties of the Ir sublattice. We deduce a markedly nonmonotonic $P$-dependence of the critical transition temperature to the antiferromagnetic state ($T_N$) hinting at its departure from $T_{MI}$. The behavior recently reported for $T_N$ from relativistic LDA+DMFT calculations closely reproduces our data under the assumption that $P$ influences the $U/W$ ratio ($U$ and $W$ representing the Coulombic repulsion and electronic bandwidth, respectively). Our $\mu$SR data confirm that the Ir$^{4+}$ magnetic moment and/or the local magnetic configuration are only weakly perturbed by pressure in the $P < 24$ kbar range. Accordingly, our measurements strongly support the preservation of a 4-in/4-out ground state.

We also report on our recent study of the pyrochlore series (Eu$_{1-x}$Bi$_x$)$_2$Ir$_2$O$_7$ for polycrystalline samples for $0 \leq x \leq 1$ [2]. We show that the lattice undergoes an anomalous contraction for $x \leq 0.05$ but that the magnetic all-in/all-out state remains robust in that limit of chemical dilutions. For small $x$ values, the resistivity approaches a $1/T$ dependence at low temperatures, suggesting a proximity to the Weyl semimetallic phase, as predicted theoretically. At $x = 0.1$ a qualitatively new ground state emerges, which is characterized by a metallic behaviour and absence of magnetic ordering at least down to 20 mK. For higher Bi-doping values, the resistivity remains metallic and it evolves gradually from $T$-like to $T^2$-like and, eventually, to $T^{3/2}$-like, suggesting the possibility of a variety of novel exotic phases.

June 14 (Fri)

Oral Presentation
Suppression of Antiferromagnetic Spin Fluctuations by Electron Doping in T’-Pr1.3-xLa0.7Ce0.3CuO4 Probed by NMR

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Electron-doped high-\(T_c\) superconducting cuprates have been studied more extensively since Matsumoto et al. reported that an adequate annealing process, which removes apical oxygens in samples, enlarges the superconducting region and reduces the antiferromagnetic (AF) region [1]. Here we report the doping dependence of AF spin fluctuations in T’-Pr1.3-xLa0.7Ce0.3CuO4 (T’-PLCCO). We performed NMR measurements of T’-PLCCO (800°C reduced samples of \(x = 0.00, 0.05, 0.10, 0.15\) and a dynamic annealed sample of \(x = 0.15\)). The previous study revealed the existence of AF spin fluctuations in T’-PLCCO (an 800°C reduced sample of \(x = 0.15\)) [2]. The temperature dependence of the spin-lattice relaxation time multiplied by temperature \(T_1T\) of T’-PLCCO is depicted in the figure. Using the Curie-Weiss-like fitting, \(T_1T = a(T+\theta)\), originating from the self consistent renormalization theory [3], it is clearly found that the AF spin fluctuations in T’-PLCCO are suppressed by electron doping.

![Figure 1: Temperature dependence of the spin-lattice relaxation time multiplied by temperature \(T_1T\) of the 800°C-reduced samples of T’-Pt1.3-xLa0.7Ce0.3CuO4+δ (T’-PLCCO) (x = 0.00, 0.05, 0.10 and 0.15) and the dynamic-annealed T’-PLCCO (x = 0.15). Solid lines denote the fitted results of the Curie-Weiss-like fitting described in the text.](image-url)

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Electron doping in the undoped (Ce-free) superconductor
\(T''-\text{La}_{1.8}\text{Eu}_{0.2}\text{CuO}_4\)

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The superconductivity in undoped (Ce-free) \(\text{Ln}_2\text{CuO}_4\) (\(\text{Ln}\): lanthanide elements) with the Nd\(_2\text{CuO}_4\)-type (so-called \(T''\)-type) structure emerges via the adequate reduction annealing without the substitution of Ce for \(\text{Ln}\), namely, without extra electron doping [1-2]. In the polycrystalline bulk sample of \(T''-\text{La}_{1.8}\text{Eu}_{0.2}\text{CuO}_4\), we have also observed the undoped superconductivity and found that the superconducting transition temperature, \(T_c\), decreases by the hole doping in polycrystalline bulk samples of \(T''-\text{La}_{1.8-x}\text{Eu}_{0.2}\text{M}_x\text{CuO}_4\) \((\text{M} = \text{Sr}, \text{Ca})\) [3,4]. Although the carrier-concentration dependence of \(T_c\) should be clarified for the investigation of the mechanism of the superconductivity, we have not succeeded in the electron doping to \(T''-\text{La}_{1.8}\text{Eu}_{0.2}\text{CuO}_4\) by the Ce substitution to La.

Here, we have succeeded in synthesizing the electron-doped polycrystalline bulk samples of \(T''-\text{La}_{1.8}\text{Eu}_{0.2}\text{CuO}_4\text{yF}_y\) \((y = 0-0.15)\) by the fluorination of \(T''-\text{La}_{1.8}\text{Eu}_{0.2}\text{CuO}_4\) using \(\text{NH}_4\text{F}\). The magnetic susceptibility measurements have revealed that \(T_c\) increases with increasing \(y\), exhibits the maximum of \(\sim 23\text{ K}\) at \(y = 0.025\), and decreases, as shown in Fig. 1. Such a dome-like dependence of \(T_c\) on the carrier concentration is explained in terms of the pairing mediated by spin fluctuations based on the \(d-p\) model calculation [5].

![Figure 1](image)

Figure 1: Carrier-concentration dependence of critical temperature, \(T_c\), for \(T''-\text{La}_{1.8-x}\text{Eu}_{0.2}\text{M}_x\text{CuO}_4\) \((\text{M} = \text{Sr}, \text{Ca})\) [3,4] and \(T''-\text{La}_{1.8}\text{Eu}_{0.2}\text{CuO}_4\text{yF}_y\). Solid lines are guides to eyes.

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Engineering the Mott State of Cuprates for High-Temperature Superconductivity

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Recent synchrotron (RIXS and ARPES) experiments on La-based cuprates will be presented [1-4]. The talk is taking basis on the recent identification of the dz2 band in overdoped La2-xSrxCuO4 (LSCO) [1]. Implications on superconductivity and pseudogap physics from of the resulting the Fermi surface structure (in- and out-of-plane) and orbital hybridization will be discussed. Topological aspects of the LSCO is being touch briefly [3]. Finally, the engineering of this electronic structure let us to find that the magnetic exchange interaction in La2CuO4 films can be tuned through strain [4]. We noticed that films with the largest exchange interaction also has the highest superconducting transition Tc upon doping – consistent with a magnetic pairing scenario.

References

Superconductivity drives magnetism in $\delta$-doped $\text{La}_2\text{CuO}_4$

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The understanding of the interplay between different orders in a solid is a key challenge in highly correlated electronic systems. In real systems this is even more difficult since disorder can have a strong influence on the subtle balance between these orders and thus can obscure the interpretation of the observed physical properties. Here we present a study on $\delta$-doped $\text{La}_2\text{CuO}_4$ ($\delta$-LCO$_N$) superlattices. By means of molecular beam epitaxy whole $\text{LaO}_2$-layers were periodically replaced through SrO$_2$-layers providing a charge reservoir, yet reducing the level of disorder typically present in doped cuprates to an absolute minimum. The induced superconductivity and its interplay with the antiferromagnetic order is studied by means of low-energy $\mu$SR. We find a quasi-2D superconducting state which couples to the antiferromagnetic order in a non-trivial way. Below the superconducting transition temperature, the magnetic volume fraction increases strongly. The reason could be a charge redistribution of the free carriers due to the opening of the superconducting gap which is possible due to the close proximity and low disorder between the different ordered regions.

Figure 1: Sketch of delta doped $\text{La}_2\text{CuO}_4$ for $N = 11$. Starting from $\text{La}_2\text{CuO}_4$, a superlattice is formed by replacing single layers of $\text{LaO}$ with SrO planes.
Uniaxial pressure control of competing orders in the cuprates

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External control of electronic phases in correlated-electron materials is a long-standing challenge of condensed-matter research. Layered cuprates exhibit antiferromagnetic, charge-density-wave (CDW), and high-temperature superconducting ground states which can be tuned by doping and external magnetic fields. However, disorder generated by lattice defects and randomly pinned magnetic vortices greatly complicates the interpretation of these experiments.

Here, we report a high-resolution inelastic x-ray scattering study of the high-temperature superconductor YBa\textsubscript{2}Cu\textsubscript{3}O\textsubscript{6.67} under uniaxial stress, and show that a three-dimensional long-range-ordered CDW state can be induced by pressure along the a-axis, in the absence of magnetic fields. The amplitude of the CDW is strongly suppressed below the superconducting transition temperature, indicating strong thermodynamic competition with superconductivity. We also show that the transition is driven by the complete softening of an optical phonon mode.

The results provide new insights into the anomalous normal-state properties of high-temperature superconductors and illustrate the potential of uniaxial-pressure control of competing orders in quantum materials \cite{1}.

Probing CDW phenomena and charge excitations in cuprates via RIXS

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Characterizing low energy excitations, in particular those associated with phonon and charge degrees of freedom, are essential to understand the rich phenomena in cuprate superconductors. In this presentation, I will first highlight our recent RIXS studies on the CDW phenomena in Bi-based double-layered cuprates. Intriguing interplay between CDW, CDW excitations, and phonon excitations as a function of temperature and doping were observed and will be discussed [1, 2]. In the second part of my talk, I will also highlight the observation of rapidly dispersed charge excitations in the electron-doped cuprates, which bear signature of plasmonic behaviors in layered 2D systems [3].

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2) H. Lu et al., in preparation.
Dual structure in the charge excitation spectrum of electron-doped cuprates

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For electron-doped cuprates, charge order and high-energy charge excitations are observed by resonant x-ray scattering (RXS) [1,2] and resonant inelastic x-ray scattering (RIXS) [3,4,5], respectively. Motivated by these experiments, we study the charge excitation spectrum of the layered $t$-$J$ model with long-range Coulomb interaction [6]. We find that the charge excitation spectrum is characterized by a dual structure in energy space. Bond-charge fluctuations driven by the exchange term ($J$ term) are responsible for the low-energy excitations, whereas the high-energy spectrum is dominated by usual on-site charge fluctuations, which yield plasmon excitations above the particle-hole continuum. We discuss that the charge order observed by RXS [1,2] can be bond-charge order characterized by $d$-wave symmetry [7, 8] and the RIXS spectrum around in-plane momentum $(0,0)$ [3,4,5] can correspond to plasmons [9, 10].

3) W. S. Lee et al., Nat. Phys. 10, 883 (2014).
7) H. Yamase, M. Bejas, and A. Greco EPL, 111 57005 (2015).
Three-dimensional Fermi surface of overdoped La-based cuprates


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The nature of the pseudogap in cuprates remains an outstanding issue. Recently, a connection between van-Hove singularity (VHS) and pseudogap collapse as a function of doping has been proposed both experimentally [1] and theoretically [2]. In this scenario, pseudogap exists only on a hole-like Fermi surface and vanishes when the Fermi surface turns electron-like with hole overdoping. In La-based cuprates, it is known that around this doping the electronic specific heat is dramatically enhanced [3,4]. This enhancement could be a signature of quantum criticality associated with the pseudogap collapse, but could also arise simply from VHS density-of-states (DOS) divergence. The latter scenario is expected to be significant in quasi-two-dimensional band structure where the VHS is well defined. It has thus become important to experimentally determine the band dispersion of La-based cuprates in a three-dimensional momentum space.

We have performed soft x-ray angle-resolved photoemission spectroscopy (ARPES) measurements on overdoped La-based cuprates La$_2-x$Sr$_x$CuO$_4$ and Eu$_0.2$La$_{1.8-x}$Sr$_x$CuO$_4$, and investigated the band structure over several Brillouin zones [5]. While nodal part of the Fermi surface was $k_z$ independent, significant $k_z$-dispersion was observed in the antinodal portion. To our knowledge, this is the first experimental observation of three-dimensional Fermi surface in La-based cuprates. From the band structure fitted to the tight-binding model, we have demonstrated that the significant $k_z$ dispersion suppresses the DOS enhancement, and thus the VHS cannot account for the large enhancement of the electronic specific heat. Our results, therefore, support quantum criticality of the pseudogap collapse as a tangible explanation for the specific heat enhancement.

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\(\pi\)-tons – generic optical excitations of correlated systems

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The interaction of light with solids gives rise to new bosonic quasiparticles, with the exciton being the most famous of these polaritons. While excitons are the generic polaritons of semiconductors, we show that for strongly correlated systems another polariton is prevalent – originating from the dominant antiferromagnetic or charge density wave fluctuations in these systems. As these are usually associated with a wave vector \(k = (\pi, \pi, \ldots)\) or close to it, we called the derived polaritons \(\pi\)-tons. These \(\pi\)-tons yield the leading vertex correction to the optical conductivity in all correlated models studied: the Hubbard, the extended Hubbard model, the Falicov-Kimball, and the Pariser-Parr-Pople model, both in the insulating and in the metallic phase [1].

The applied parquet equation methods: parquet dynamical vertex (D\(\Gamma\)A) and parquet approximations, implemented within the \textit{victory} code [2], as well as the parquet dual fermion (DF) method, allow for unbiased study of contributions from different channels. The diagrammatic decomposition of the results enables the analysis of the underlying physical processes.

![Figure 1](image.png)

Figure 1: Sketch of the physical processes (top) and Feynman diagrams (bottom) behind an exciton (left) and a \(\pi\)-ton (right). The yellow line symbolizes the incoming (and outgoing) photon which creates an electron-hole pair denoted by open and filled circles, respectively. The Coulomb interaction between the particles is symbolized by a red wiggled line; black lines in the top part denote the underlying band-structure.

Spontaneous Magnetic Field near a Time-Reversal Symmetry Broken Surface State of YBCO

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Spatial distributions of spontaneous magnetic fields, $\mathbf{B}$, near a (110) surface of cuprate high-$T_C$ superconductor YBCO with broken time-reversal symmetry are calculated, using the Ginzburg-Landau theory derived from the $t-J$ model. Considering a system with infinite stacking of CuO$_2$ bilayers, we show the spatial variations of the in-plane ($B_x$) and vertical ($B_z$) components of $\mathbf{B}$ as functions of the distance from the surface, $x$, in Fig.1. (Here, the $x$ axis is taken to be perpendicular to the surface.) It is seen that $\mathbf{B}$ exists only in the region within the superconducting coherence length $\xi_d$ from the surface. Outside the surface, magnetic fields decay quickly, and the typical length scale for the decay is of the order of $c_1$, the distance between bilayer (a few Å).

Since the magnetic field exists essentially inside the superconductor, it would be difficult to detect it using, e.g., SQUID microscope. Experimental approaches possible to measure it may be $\mu$SR or polarized neutron scattering.

![Figure 1: Spatial variations of $B_z$ and $B_x$. $z = 0$ corresponds to the center of a bilayer, and $c_1$ is the distance between two layers.](image)

ARPES studies of electronic nematic phases in cuprate and iron-based superconductors

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The microscopic origin of the pseudogap in cuprates has been a long standing mystery [1]. In recent years, spontaneous breaking of the four-fold rotational symmetry of the electronic system, that is, so-called electronic nematicity was observed by magnetic and transport measurements [2].

We performed ARPES measurements on slightly overdoped Pb-Bi2212 under uniaxial strain, and observed the four-fold rotational symmetry breaking of the Fermi surface only in the pseudogap phase [3]. If the nematicity is a purely \( Q = 0 \) instability, it cannot open a gap since there is no band folding nor nesting. Therefore, the observation that the nematic transition and the pseudogap opening occur simultaneously at \( T^* \) [2] suggest that the nematicity is not the origin of the pseudogap but is somehow caused by the pseudogap opening. Alternatively, the nematic state may be a \( Q \neq 0 \) density-wave ordered state [4], but the effect of the density wave is too weak to observe by ARPES.

The nematicity of Fe-based superconductors above the magneto-structural transition temperature [5] has been observed by many ARPES studies under uniaxial strain, too [6], and has been attributed to a ferro-orbital order. In addition to the strong nematic signal (inequivalent band structures between the \( k_x \) and \( k_y \) directions), we observed a signature of \( Q \neq 0 \) band folding above the magneto-structural transition in BaFe₂As₂ [7], suggesting a superposition of ferro- and antiferro-orbital orders. This suggests that density waves (\( Q \neq 0 \)) open a gap and also drive the nematicity (\( Q = 0 \)) [4].


3) S. Nakata et al., arXiv:1811.10028.
7) K. Koshiishi, Thesis (University of Tokyo, 2019).
Nematic fluctuation and resonance in BaFe$_2$(As,P)$_2$ observed by Raman scattering spectroscopy

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Various iron-based superconductors show the in-plane anisotropy of the electronic properties, so-called “electronic nematicity” above the structural/magnetic transition temperature ($T_s$) [1-3]. Its origin and relationship with the superconductivity have been intensively debated, but they still remain unclear. Raman scattering spectroscopy is a powerful tool to investigate the electronic properties in solid. In particular, its symmetry-resolved feature enables us to directly access the bare electronic nematic behavior [4,5]. In this work, we have investigated the doping dependence of the nematic Raman response for P-doped Ba122 system, BaFe$_2$(As$_{1-x}$P$_x$)$_2$.

The nematic susceptibility has been estimated from the quasi-elastic peak of B$_{1g}$ Raman scattering spectra, and its temperature dependence can be fitted by the Curie-Weiss law. The nematic fluctuation temperature $T^*$ is determined as the starting temperature of the enhancement of the nematic susceptibility. $T^*$ is higher than $T_s$ and systematically decreases with increasing P doping level. On the other hand, the Curie-Weiss temperature is the bare nematic transition temperature $T_0$. $T_0$ also decreases with P doping and becomes 0 K very near the magnetic/structural quantum critical point (QCP). This result has indicated that the nematic QCP exists near magnetic/structural QCP and near optimally doping region ($x$~0.30) for superconductivity in the phase diagram of P-doped Ba122 system.

In the superconducting state, the pair breaking peaks have been observed in A$_{1g}$ and B$_{1g}$ Raman scattering spectra. In addition, the nematic resonance peak with large intensity appears below the superconducting transition temperature in Raman scattering spectrum with B$_{1g}$ symmetry only in the optimally doped sample. The energy of the nematic resonance peak is slightly lower than the pair breaking peak energy. The existence of a clear nematic resonance peak suggests the remarkable correlation between the superconductivity and the nematic fluctuation.

5) Y. Gallais and I. Paul et al., C. R. Physique 17, 113 (2016).
Quest for the origin of various nematicities in Fe-based superconductors

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The superconducting phase is adjacent to the nematic phase in Fe-based superconductors. The origin of the superconductivity would be closely related with the nematic state. Thus, the origin and nature of nematic phenomena are the central issues in Fe-based superconductors. We explained that the origin of the $B_{1g} (=d_{x^2-y^2})$ nematic order in the non-doped ($n_d = 6$) systems is the ferro orbital order by using the Aslamazov-Larkin vertex correction (AL-VC) theory [1]. The AL-VC theory describes the strong interference between charge and spin fluctuations.

Recently, however, a new type of nematic order/fluctuation with $B_{2g} (=d_{xy})$ symmetry, rotated by $45^\circ$ from the conventional $B_{1g}$ nematicity, has been discovered in heavily hole-doped ($n_d = 5.5$) compound AFe$_2$As$_2$ (A=Cs, Rb)[2-4]. To reveal the origin of the $B_{2g}$ nematicity, we investigate the spontaneous symmetry-breaking in the self-energy $\Delta \Sigma$ using the CDW equation based on the AL-VC theory [5,6]. We predict that the $B_{2g}$ nematic bond order, which is given by the symmetry-breaking of the next-nearest-neighbor correlated hopping, is the origin of $B_{2g}$ nematic order in AFe$_2$As$_2$.

In BaFe$_2$As$_2$, nematicity starts to develop at $T = T^*$ [7], which is higher than the $B_{1g}$ structural phase transition temperature $T_S$. The origin of the nematicity at $T^*$ is a long standing unsolved problem. Both the extrinsic origin due to the local uniaxial strain and the intrinsic origin due to another phase transition have been proposed. In addition, the pseudogap in the density of states is observed below $T^*$ [8]. We predict that the origin of the nematicity below $T^*$ is the antiferro charge nematic order by solving the CDW equation based on the AL-VC theory. The $T$-linear behavior of $a - b \propto n_{xz} - n_{yz}$ below $T^*$ [7] and the emergence of pseudogap [8] are naturally explained by the antiferro charge nematic order. The antiferro charge nematic fluctuation would favor the $S_{++}$ wave superconductivity without sign reversal.

The variety of nematicity in Fe-based superconductors is naturally understood by the AL-VC theory.

2) J. Li et al., arXiv:1611.04694.
3) X. Liu et al., arXiv:1803.07304.
4) K. Ishida et al., arXiv:1812.05267.
Infrared Spectroscopic Studies of the Phonon Dynamics in Iron-based Superconductors

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The temperature dependence optical reflectivity has been measurement on iron-based superconductors of different families. The optical conductivity has been obtained by using the two-Drude component model. It has been found that the phonons show red- or blue-shift in different samples. Interestingly, the phonon conductivity exhibits a Fano lineshape, suggesting possible coupling between phonon and electrons or spin. Based on the temperature evolution of the lineshape and peak shift, we discuss the possible role played by electron-phonon and spin fluctuation in the occurrence of superconductivity in iron-based superconductors.
High-Tc superconductivity in absence of nematic fluctuations in CaKFe$_4$As$_4$

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Understanding the pairing mechanism in the Fe-based superconductors (FeSCs) remains in focus of research not only due to a high superconducting transition temperature $T_c$, but also because of the interplay of superconductivity with other electronic degrees of freedom, nematicity and magnetism in particular. Electronic nematicity has been universally observed for many families of FeSCs. Furthermore, compositions that are in proximity to the nematic quantum critical point often show the highest $T_c$.

A new class of stoichiometric and strictly tetragonal superconductors CaAFe$_4$As$_4$ (A = K, Rb, Cs) with rather high $T_c$ (31-36 K) provides an ideal platform for spectroscopic investigation of FeSCs in a clean limit, and to decide if the nematicity is a necessary condition for high-Tc superconductivity in FeSCs.

We employ polarization-resolved Raman spectroscopy to study superconductor CaKFe$_4$As$_4$ with $T_c = 35$ K. We do not detect electronic nematic fluctuations which were observed in XY ($B_{2g}$) symmetry Raman response for most families of the Fe-based superconductors. In the superconducting state, we observe the development of a composite coherence feature between 12 and 20 meV and a complete suppression of low-frequency spectral weight in the $B_{2g}$ symmetry channel, which implies that all the FS pockets remain nodeless. We also study the SC-induced self-energy effects for Raman-active phonons and provide an estimate of the electron-phonon coupling constant $\lambda^f = 0.0015$, which is very small for a superconductor with $T_c$ at 35 K [1].

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The iron-based superconductor FeSe has attracted special attention because it uniquely has a pure nematic phase without a magnetic ordering. It is considered as a key material for investigating the influence of nematicity on superconductivity. The superconducting state inside the nematic phase also has unique properties, and it has been recently proposed that the superconducting order parameter breaks the time-reversal symmetry near the nematic twin boundaries. The lifting of superconducting gap nodes due to twin boundaries has been observed in scanning tunneling spectroscopy [1] and angle-resolved photoemission spectroscopy [2], which is consistent with the induced imaginary component. However, these measurements of the gap structure provide only indirect evidence for time-reversal symmetry breaking (TRSB), and thus the observation of spontaneous internal magnetic field generated by TRSB is indispensable. Here we report on the zero-field muon spin rotation ($\mu$SR) measurement, which is one of the most sensitive magnetic probes, in high-quality single crystals of FeSe. We find that the relaxation rate starts to grow just below $T_c$ (=9 K). This indicates that weak but finite internal magnetic field is induced in the superconducting state, providing strong evidence for TRSB state in FeSe.

Nature of zero-energy vortex bound state in superconducting topological surface state of Fe(Se,Te)

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Vortex cores of topological superconductors are predicted to be an ideal platform of Majorana fermions. Although several experimental efforts have been made to detect Majorana fermions in the vortex cores as a zero-energy vortex bound state (ZVBS) [1-3], existence of the Majorana fermions is still controversial [4]. Using a dilution-refrigerator scanning tunneling microscope [5], we have systematically examined a large number of vortices in the superconducting topological surface state of FeTe₀.₆Se₀.₄ with unprecedentedly high energy resolution of ~20 \( \mu \text{eV} \). We found that a certain number of vortices possess the ZVBS below 20 \( \mu \text{eV} \), which suggests its Majorana bound-state origin. However, we also found vortices without the ZVBS. Interestingly, emergence of the ZVBS is not related to the preexisting quenched disorders, and the fraction of vortices with the ZVBS decreases with increasing magnetic field [6]. These findings suggest that inter-vortex interaction plays an important role in the ZVBS formation.

![Figure 1.](image_url)

Figure 1. (a) A zero bias conductance map in a 187 nm x 187 nm field of view of a set point at \( V = -10 \) mV and \( I = 100 \) pA. (b) and (c) Line profiles of high energy resolution tunneling spectra across the vortex core with and without the ZVBS, respectively.

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4) M. Chen et al., Nature Commun. 9, 970 (2018)
We show that multiband superconductors with dominant spin singlet, intraband pairing of spin-1/2 electrons can undergo a transition to a state with Bogoliubov Fermi surfaces -- surfaces of zero energy excitations that are topologically protected in the superconducting state -- if spin-orbit coupling, interband pairing and time reversal symmetry breaking are also present. These latter effects may be quite small, but still drive the transition to the topological state if the nodal structure of the intraband pairing is appropriate. Such a state should display a nonzero zero-bias density of states and corresponding residual Sommerfeld coefficient as for a disordered nodal superconductor but occurring even in the pure case. We present a model appropriate for iron-based superconductors where the topological transition associated with the creation of a Bogoliubov Fermi surface can be studied. The model gives results that strongly resemble experiments on FeSe$_{1-x}$S$_x$ across the nematic transition, where this \textquotedblleft ultranodal\textquotedblright behavior may already have been observed.
June 15 (Sat)

Oral Presentation
Insulating Parent Phase and Distinct Doping Evolution to Superconductivity in Single-Layer FeSe/SrTiO$_3$ Films

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The single-layer FeSe/SrTiO$_3$ (FeSe/STO) films have attracted much attention because of their simple crystal structure, distinct electronic structure and record high superconducting transition temperature ($T_c$). The origin of the dramatic $T_c$ enhancement in single-layer FeSe/STO films and the dichotomy of superconductivity between single-layer and multiple-layer FeSe/STO films are still under debate. In this talk, I will report a comprehensive high resolution angle-resolved photoemission spectroscopy and scanning tunneling microscopy/spectroscopy measurements on the electronic structure evolution with doping in single-layer and multiple-layer FeSe/STO films. We find that the single-layer FeSe/STO films have distinct parent phase and route of doping evolution to superconductivity that are fundamentally different from multiple-layer FeSe/STO films. The parent phase of the single-layer FeSe/STO films is insulating, and its doping evolution is very similar to doping a Mott insulator in cuprate superconductors. In multiple-layer FeSe/STO films, high temperature superconductivity occurs by suppressing the nematic order in the parent compound with electron doping. The single-layer FeSe/STO films represent the first clear case in the iron-based superconductors that the parent compound is an insulator. Our observations of the unique parent state and its doping evolution in the single-layer FeSe/STO films provide key insight in understanding its record high-$T_c$ superconductivity. They also provide a new route of realizing superconductivity in iron based superconductors which is similar to that in high temperature cuprate superconductors.

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Superconductivity and fermiology in atomically-thin iron-chalcogenide films studied by ARPES

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The discovery of high-temperature ($T_c$) superconductivity above 65 K in monolayer FeSe film on SrTiO$_3$ substrate (Fig. 1) [1] has generated tremendous attention because the $T_c$ value is surprisingly high and the material is an atomically thin (a few angstrom thick) film. While previous studies suggested the importance of interfacial effects, e.g., electron charge transfer [2-4] and interfacial electron-phonon coupling [5], the origin of the observed drastic $T_c$ enhancement in monolayer FeSe is still under intensive debate. To clarify this issue, a comparative study on monolayer films of various iron-based superconductors would be of crucial importance.

In this study, we have fabricated chalcogen-substituted monolayer films on SrTiO$_3$ substrate by molecular-beam epitaxy technique and determined the electronic structure by using high-resolution angle-resolved photoemission spectroscopy (ARPES). We observed substitution-induced changes in the $T_c$ value, Fermi-surface shape, and band width. We also detected a signature of interfacial electron-phonon coupling. We discuss the implications of our ARPES results in relation to the high-$T_c$ mechanism of atomically-thin iron-based superconductors.

Figure 1: Schematic view of monolayer FeSe film on SrTiO$_3$ substrate.

2) S. He et al., Nat. Mater. 12, 605 (2013).
3) S. Tan et al., Nat. Mater. 12, 634 (2013).
Comparison between Te- and S-substitution effects on superconductivity in FeSe thin films

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We grew single crystalline films of FeSe₁₋ₓSₓ with x ≤ 0.43 via pulsed laser deposition. As x increases, the structural transition temperature decreases and the superconducting transition temperature, T_c, shows a gradual decrease even when the structural transition disappears. We observed a new kink structure in the resistivity-temperature curves for films with large x, which is likely due to a magnetic transition. The obtained phase diagram of FeSe₁₋ₓSₓ is similar to that of bulk FeSe₁₋ₓSₓ except for the possible magnetic transition, but is in contrast to that of FeSe₁₋ₓTeₓ films, which shows a sudden increase of T_c at the composition where the structural transition disappears¹). These results suggest that the nematicity has no universal significance on the superconductivity in FeSe²). A systematic magneto-transport study revealed a positive correlation between carrier densities and T_c in these films. These results suggest that the structural transition affects the electronic structure differently between Fe(Se,S) and Fe(Se,Te) and that this is the direct cause of the difference in the T_c behaviors at the end point of the structural transition.

Figure 1: Schematic phase diagram of S- and Te-substituted FeSe thin films. T* represents possible magnetic transition temperature.

Ultrafast nematic-orbital excitation in FeSe

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The electronic nematic phase is an unconventional state of matter that spontaneously breaks the rotational symmetry of electrons[1]. In iron-pnictides/chalcogenides[2] and cuprates[3], the nematic ordering and fluctuations have been suggested to have as-yet-unconfirmed roles in superconductivity. However, most studies have been conducted in thermal equilibrium[4], where the dynamical property and excitation can be masked by the coupling with the lattice. Here we use femtosecond optical pulse to perturb the electronic nematic order in FeSe. Through time-, energy-, momentum- and orbital-resolved photo-emission spectroscopy, we detect the ultrafast dynamics of electronic nematicity[5]. In the strong-excitation regime, through the observation of Fermi surface anisotropy, we find a quick disappearance of the nematicity followed by a heavily-damped oscillation. This short-life nematicity oscillation is seemingly related to the imbalance of Fe 3$d_{xz}$ and $d_{yz}$ orbitals. These phenomena show critical behavior as a function of pump fluence. Our real-time observations reveal the nature of the electronic nematic excitation instantly decoupled from the underlying lattice.

5) T. Shimojima et al., Nat. Commun. Accepted.
Dynamical magnetism in iron-based ladder compounds

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Since the discovery, iron-based superconductivity (SC) has attracted much attention. Interplay between structure, magnetism and SC is one of most intriguing subjects of this research field. To gain further insight into the mechanism of SC, investigation of iron-based compounds over distinct spatial dimensions is important. This is because the dimensionality strongly influences magnetism and can control itinerancy of electrons by changing Fermi surface topology.

We have thus examined magnetism of iron-based ladder compounds AFe$_2$X$_3$ (A = Rb, Cs, Ba; X = S, Se) [1,2]. This is known as the one-dimensional analogue of the iron-based superconductors, and we have recently found the first superconductivity in BaFe$_2$S$_3$ by applying pressures [3]. In the ladder compounds, crystal structure consists of FeX$_4$ tetrahedra with channels that host A cations. Four-fold coordinated Fe$^{2+}$ ions extend and forms two-leg ladder structure. As for parent compounds of the iron-based superconductors, this family shows three-dimensional magnetic ordering. However, most of bulk properties measurements are not sensitive to the magnetic transition.

For BaFe$_2$Se$_3$ as an example, Block-type magnetic structure below $T_N = 255$ K was clarified by neutron diffraction [1]. However, Mössbauer experiment reports no anomaly at $T_N$, instead hyperfine splitting appears below 235 K. This separate behavior can be originating from the difference in timescale of the techniques; neutrons typically have $10^{-13}$ to $10^{-12}$ sec timescale, being faster than Mössbauer ($10^{-7}$ sec). Mössbauer signal infers a coexisting of paramagnetic and magnetically ordered phase even below 235 K, and the magnetic order gradually forms with decreasing temperature. It could finally fall into the quasi-static state at 10 K.

Here we report on magnetic dynamics of BaFe$_2$Se$_3$ and related compounds elucidated through multi-probe techniques. Combining inelastic neutron scattering, neutron spin echo and muon spin relaxation, we provide evidence for slowing down of magnetic fluctuations over a wide regime of temperature. We argue such slow spin dynamics is inherent to low-dimensional ladder geometry of the material.


Exploration of Novel Pt-based Superconductors with Honeycomb Networks

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Alkaline-earth platinum pnictides exhibit a variety of hexagonal structures that are characterized by honeycomb networks, such as CaPt$_2$P$_2$, SrPtAs, and BaPtSb with an AlB$_2$-($P6/mmm$, $D_{6h}^1$, No. 191), a KZnAs-($P6_3/mmc$, $D_{6h}^4$, No. 194), and a SrPtSb-type($P-6m2$, $D_{3h}^1$, No. 187) structures, respectively. SrPtAs with a PtAs ordered honeycomb network exhibits superconductivity at the transition temperature $T_c$ of 2.4 K, as we reported [1]. Superconductors with honeycomb networks have attracted interest since the theoretical predictions of exotic superconductivity in SrPtAs, such as a singlet-triplet mixed state [2], a chiral $d$-wave state [3], and an $f$-wave state [4]. In order to explore the exotic superconducting states, we have developed novel compounds with honeycomb networks.

In this talk, we will report on the discovery of superconductivity in BaPtAs and BaPtSb with PtAs and PtSb ordered honeycomb networks, respectively. BaPtSb exhibited superconductivity at 1.64 K [5]. The muon spin rotation/relaxation measurements showed a slight increase in the relaxation rate of muon spins below $T_c$. The result has suggested the occurrence of a spontaneous magnetic field below $T_c$ and thus the chiral $d$-wave state as a possible superconducting state [6]. On the other hand, BaPtAs was known as a cubic LaIrSi-type compound. We have discovered the hexagonal structures of BaPtAs, namely, SrPtSb-($P-6m2$, $D_{3h}^1$, No. 187) and YPtAs-type($P6_3/mmc$, $D_{6h}^4$, No. 194) structures [7]. Both structural phases exhibited superconductivity at 2.8 and 2.1-3.0 K, respectively [7]. Inversion symmetry is broken in the SrPtSb-type, whereas it is preserved in the YPtAs-type. Our discovery provides opportunities not only for the experimental examination of the predicted superconductivity but also for further studies on exotic states that result from the strong spin-orbit interaction of Pt under broken inversion symmetry.

This work was conducted in collaboration with M. Nohara, Y. Saito, T. Takeuchi, H. Ota (Okayama University), and T. Adachi (Sophia University).

Observation and control of nematic superconductivity in doped Bi$_2$Se$_3$ topological superconductors

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Topological superconductivity, accompanying non-trivial topology in its superconducting wave function, has been one of the central topics in condensed-matter physics. During the recent extensive efforts to search for topological superconducting phenomena, nematic superconductivity, exhibiting spontaneous rotational symmetry breaking in bulk superconducting quantities, has been discovered in the topological-superconductor candidates A$_x$Bi$_2$Se$_3$ ($A =$ Cu, Sr, Nb) [1] (Fig. 1). In the in-plane field-angle dependence of various superconducting properties, such as the spin susceptibility measured using nuclear magnetic resonance [2], the specific heat [3], and the upper critical field [4], exhibit pronounced two-fold symmetric behavior although the underlying lattice has three-fold rotational symmetry. More recently, microscopic evidence for nematic superconductivity, such as two-fold elongation of vortex cores, has been found using scanning tunneling microscopy/spectroscopy [5].

In this talk, I overview recent experiments on nematic superconductivity with some focus on our specific-heat study [3], and explain our recent attempts to control nematic superconductivity.

This work has been performed under collaboration with Y. Maeno, K. Tajiri, I. Kostylev, R. Taniguchi, S. Nakata (Kyoto Univ., Japan), Y. Ando, Z. Wang (Univ. Koeln, Germany), K. Segawa (Kyoto Sangyo Univ., Japan), and Y. Nagai (JAEA, Japan).

Figure 1: Schematic figures of the proposed gap structures for the nematic superconducting states in A$_x$Bi$_2$Se$_3$, with horizontal cuts in the bottom row [1]. The arrows depict the $d$-vector order parameters; and the distance between the colored surface and the gray sphere explains the gap amplitude.

1) For a recent review, see S. Yonezawa, Condens. Matter 4, 2 (2019).
Effect of Antisymmetric Spin-Orbit Interaction on Critical Field of Ion-Gated 2D Superconductors

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Recently, the exotic superconducting properties have been intensively investigated in highly crystalline two-dimensional (2D) electron systems [1], which became available with the technological advances in thin film growth, exfoliation, and ionic gating. Among them, the 2D electron system induced by electric field gating is an ideal platform for non-centrosymmetric superconductivity with strong antisymmetric spin-orbit interaction (ASOI). In this presentation, I report our recent magnetotransport experiments on ion-gated SrTiO$_3$ and MoS$_2$ single crystal surfaces in electric double layer transistors (EDLTs), which show the electric-field-induced superconductivity at $T_c = 0.3 - 0.4$ K [2] and 6 -10 K [3], respectively, depending on the surface carrier density.

In both samples, the superconducting transition is extremely anisotropic against the direction of magnetic fields reflecting the 2D nature of the electron systems. Especially, the in-plane upper critical fields $H_{c2//}$ derived from the resistive transitions reach 4.3$T_c$ for SrTiO$_3$-EDLT and 8$T_c$ in MoS$_2$-EDLT [3] at low temperature, which exceed far the usual Pauli-Clogston-Chandrasekhar (paramagnetic depairing) limit of 1.8$T_c$. These phenomena can be ascribed to the different types of ASOI, (i) the Rashba-type ASOI in combination with multi-orbital effect of 3$d$ elections for EDLT-SrTiO$_3$ [4] and (ii) the intrinsic Zeeman-type SOI with in-plane broken inversion symmetry for EDLT-MoS$_2$ [3], both of which cause the enhancement of the paramagnetic limit, with the spins of Cooper pairs aligned perpendicularly to the magnetic field though the spin-momentum and spin-valley locking. I will also discuss the data of angular dependence of the upper critical field around the in-plane condition clearly deviates from the well-known Thinkham formula (description of orbital depairing limit), which can be the evidence that the critical fields in these samples are determined by the unusual paramagnetic limit enhanced by ASOI.

This work has been done in collaboration with T. Ouchi (Tohoku U.), Y. Saito (U. Tokyo, now at U. California, SB), Y. Itahashi (U. Tokyo), S. Shimizu (RIKEN, now at CRIEPI) and Y. Iwasa (U. Tokyo and RIKEN), and was supported by JSPS KAKENHI Grant Number JP15H05884 (J-physics). Part of this work was performed at High Field Laboratory for Superconducting Materials, Institute for Materials Research, Tohoku University (Project No 18H0409, 19H0409).

Fulde-Ferrell-Larkin-Ovchinnikov Phases in Layered Organic Superconductors

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In conventional superconductors, the superconducting order parameter is spatially homogeneous. However, when the superconductivity is in the clean limit and the orbital effect is strongly quenched, so-called Fulde and Ferrell, and Larkin and Ovchinnikov (FFLO) phase with an inhomogeneous order parameter can be stabilized in fields above the Pauli limit \( H_{\text{Pauli}} \). Layered organic superconductors are best candidates for the FFLO phase studies. In the FFLO phase, the order parameter is given by \( \Delta(r) = \Delta_0 \cos(qr) \), where \( q \) is the center-of-mass momentum of the Cooper pairs. When a magnetic field is applied parallel to the layers, flux lines penetrate the insulating layers, forming Josephson vortices (JVs). The JVs are easily driven by a perpendicular current, leading to nonzero interlayer resistance in the SC phase.

When the wavelength of the FFLO order parameter oscillation \( \lambda_{\text{FFLO}} = 2\pi/q \) becomes commensurate with the JV lattice constant \( l \), the JVs are collectively pinned and dips periodically appear in the field dependence of the interlayer resistance. This commensurability (CM) effect is a powerful tool to estimate the order parameter oscillation in the FFLO phase. So far, we have found the CM effects in the FFLO phases for three different layered organic superconductors [Fig. 1] [1,2]. For these superconductors, the FFLO phases appear above \( \sim H_{\text{Pauli}} \) at low temperatures. On reasonable assumptions, we can estimate \( \lambda_{\text{FFLO}} \), which decreases as the field approaches \( H_{c2} \).

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{superconducting_phase_diagrams.png}
\caption{Superconducting phase diagrams for three different organic layered superconductors. Red regions show FFLO phases.}
\end{figure}

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Collective mode of the Hidden Order State in URu$_2$Si$_2$: Degeneracy and Symmetry

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More than thirty years after the discovery of the hidden order (HO) in the heavy fermions compound URu$_2$Si$_2$, the microscopic nature of this exotic state still remains a major enigma of condensed matter research [1]. Raman scattering spectroscopy recently brought important insights on the nature of this state [2,3]. Two clear signatures of the hidden order state were measured, a peak at 14 cm$^{-1}$ and a gap below ~55 cm$^{-1}$, both in the chiral symmetry A$_{2g}$. The nature of the former mode particularly attracts attention; the temperature dependences of both its energy and width fully match the ones of the neutron resonance measured at $Q_0 = (0\ 0\ 1)$ [2], up to now the main fingerprint of the hidden order. Moreover, it has been suggested that the f-electron ground state might be a singlet $f$-state having the A$_{2g}$ symmetry [3]. However, more ground states giving also Raman excitations in the A$_{2g}$ channel are possible [4], including a E$_g$ ($\Gamma_5$) doublet, symmetry that has never been explored by Raman spectroscopy at low energy (down to 1 meV).

Here, thanks to a newly developed Raman spectroscopic set-up under high magnetic fields at the High Field Magnet Laboratory (Nijmegen, Netherlands), we report low-energy Raman spectroscopic measurements in all symmetries, including the E$_g$ one and under high magnetic fields up to 25 T. No splitting of the A$_{2g}$ collective mode is observed up to 25 T and no collective mode is found in E$_g$ symmetry around 14 cm$^{-1}$. These two results together push toward a singlet nature for the ground state of f-electrons in the HO, a key ingredient to solve the longstanding mystery of the hidden order nature.

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NMR Studies on U-based Ferromagnetic Superconductors

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Since the discovery of superconductivity in ferromagnet UGe₂ under pressure [1], U-based ferromagnetic (FM) superconductors have attracted much attention since spin-triplet superconductivity is anticipated. Within them, URhGe [2] and UCoGe [3] show superconductivity at ambient pressure, and the latter has the highest superconducting (SC) transition temperature $T_{\text{Super}} = 0.57$ K below FM ordering at $T_{\text{Curie}} = 2.5$ K.

We have studied single-crystal UCoGe with microscopic measurements of $^{59}$Co nuclear magnetic resonance (NMR) and nuclear quadrupole resonance (NQR). We showed that superconductivity occurs in the FM region [4] and that both phenomena originate from U $5-f$ electrons [5], resulting in the microscopic coexistence of ferromagnetism and superconductivity realized in UCoGe. We also studied the spin-dynamic properties from the measurements of $1/T_1$ and Knight shift along the each crystalline axis. The results show that both static and dynamic susceptibilities possess the strong Ising anisotropy along the c axis being the easy axis and that the FM fluctuations are predominant at low temperatures and persist even below $T_{\text{Curie}}$ [6]. From the angle-resolved NMR measurements, we found that the magnetic field along the c axis ($H||c$) strongly suppresses both the FM Ising-type fluctuations and superconductivity in the same manner [7]. On the other hand, we found that the field along the b axis ($H||b$) above 5 T enhances the Ising FM fluctuations at low temperatures, and that the superconductivity also becomes robust in the same field region [8]. These results strongly suggest that the characteristic FM fluctuations tuned by external fields induce unique spin-triplet superconductivity in UCoGe. This scenario is also supported by the recent $^{59}$Co-NQR/NMR measurements under pressure [9, 10], which have been performed to study the character of the transition from the FM state to the paramagnetic (PM) state [9, 10], and the properties of the superconductivity occurring in the PM state.

We will introduce NMR results on single-crystal URhGe [11, 12] and UTe₂[13], and discuss the similarity and difference in these superconductors.

References

Nonsymmorphic topological superconductivity in the paramagnetic superconducting phase of UCoGe

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Superconductivity with emergent topologically nontrivial properties, namely topological superconductivity (TSC), has attracted great attention in these days [1]. Recent studies have revealed that the presence of crystalline symmetries enriches topological structures in SCs [2]. Among them, TSC enriched by nonsymmorphic (NSM) crystalline symmetries is dubbed topological NSM crystalline superconductivity (TNCS), and takes much interest because of the novel topological structures represented by Möbius- or hourglass-shaped surface states unique to NSM systems [3-5]. Interestingly, some of TNCS are classified into $\mathbb{Z}_4$ topological phases, which do not appear in the conventional topological periodic table [1]. However, material realization of such $\mathbb{Z}_4$ TNCS has been lacking, to the best of our knowledge.

Here, we propose that the paramagnetic superconducting phase of UCoGe under pressure [6] is a promising candidate of TNCS with nontrivial $\mathbb{Z}_4$ indices. We clarify that the glide topological invariants on the Brillouin-zone faces are determined from Fermi-surface topology, and demonstrate the topological invariants take nontrivial values for Fermi surfaces of UCoGe previously obtained by ab-initio calculations [7]. We check our predictions by tight-binding model calculations, and illustrate the $4\pi$-periodic surface states.

![Figure 1: 4\pi-periodic surface states of $\mathbb{Z}_4$ TNCS.](image)

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4) Z. Wang et al., Nature 532, 189 (2016)