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

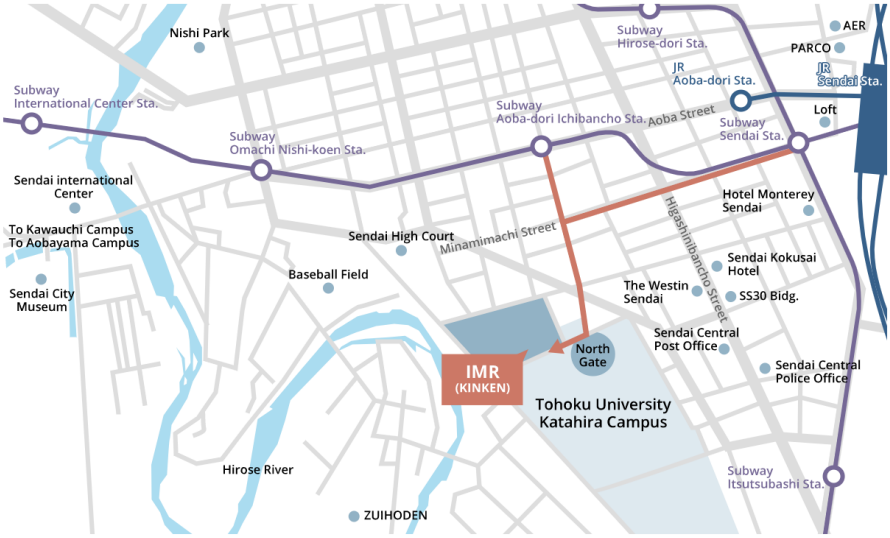
Abstract

Venue

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

Access

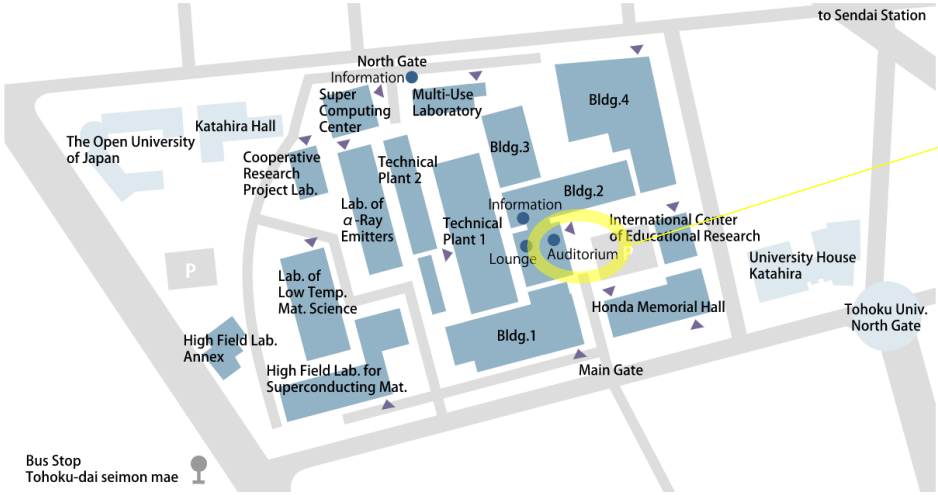
Institute for Materials Research, Tohoku University 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan



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 Superexchange 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 $Eu_2Ir_2O_7$

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'-$Pr_{1.3-x}La_{0.7}Ce_xCuO_4$ Probed by NMR

9:20 - 9:40 Takayuki Kawamata（Tohoku Univ.）
Electron Doping in the Undoped (Ce-Free) Superconductor T'-$La_{1.8}Eu_{0.2}CuO_4$

9:40 - 10:05 Johan Chang（Univ. of Zurich）
Engineering the Mott State of Cuprates for High-Temperature Superconductivity

10:05 - 10:30 Andreas Suter（PSI）
Superconductivity Drives Magnetism in δ-Doped La_2CuO_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）
π-tons - 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 $BaFe_2(As,P)_2$ 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-T_c superconductivity in Absence of Nematic Fluctuations in $CaKFe_4As_4$

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/$SrTiO_3$ 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 Bi_2Se_3 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 URu_2Si_2: 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_2CuO_{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. Grochala[1]

[1] *Centre of New Technologies, University of Warsaw, Poland*

[2] *Faculty of Mathematics and Natural Sciences, Cardinal Stefan Wyszyński University in Warsaw*

[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-T_c 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 d^9 by Ag d^9. As will be discussed, this requires replacing O by F to retain a positive charge transfer energy. AgF_2 (**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 AgF_2 planes could have an antiferromagnetic coupling that matches or surpasses the cuprates potentially leading to high-T_c superconductivity.

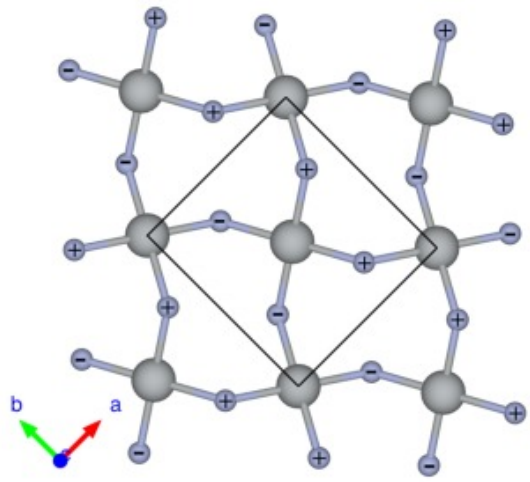


Figure 1: Schematic view of an AgF_2 plane.

1) Gawraczyński, J. *et al.,* PNAS **116** 1495 (2019).

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 $Sr_3Mo_2O_7$ and $Sr_3Cr_2O_7$ 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:

1) K. Kuroki, T. Higashida, and R. Arita, Phys. Rev B, **72**, 212509 (2005).
2) K. Matsumoto, D. Ogura, and K. Kuroki, Phys. Rev. B **97**, 014516 (2018).
3) D. Ogura, H. Aoki, and K. Kuroki, Phys. Rev. B **96**, 184513 (2017).

Self-energy variational approach to correlated electron systems

Shiro Sakai[1], Ryotaro Arita[1,2]
[1]*RIKEN Center for Emergent Matter Science, Saitama 351-0198, Japan*
[2] *Department of Applied Physics, University of Tokyo, Tokyo 113-8656, Japan*

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).

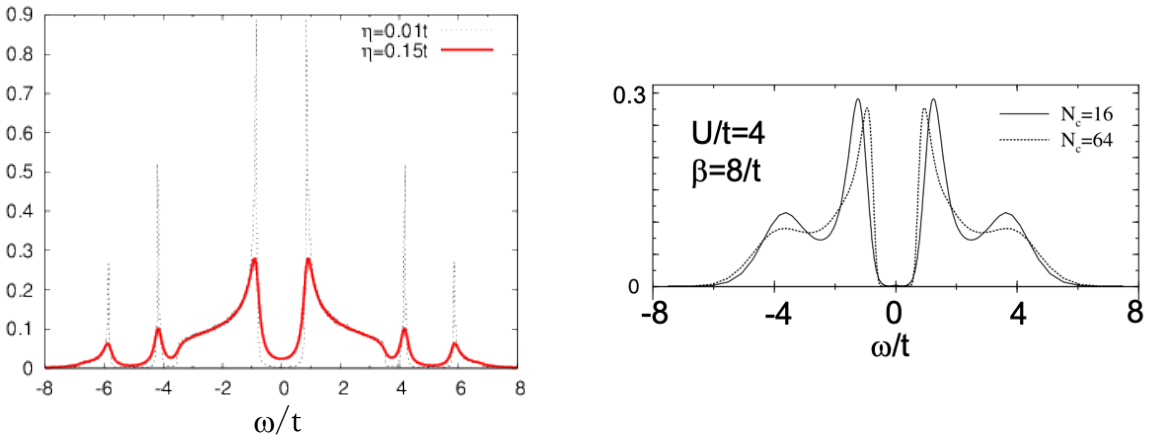


Figure 1: Spectral function of the two-dimensional Hubbard Model. We compare the results obtained by the present method (left) and Quantum Monte Carlo calculation for finite systems (right, taken from Moukouri and Jarrell, PRL 87, 167010 (2001)), where we see a good agreement.

RIXS in 4d-electron systems: Probing magnons, spin-orbit excitations, and Hund's multiplets in ruthenates

Giniyat Khaliullin
Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany

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 $SrRu_2O_6$ and Ca_2RuO_4, and show how the above interaction parameters can be extracted from the RIXS data using a simple model calculations. In quasi-two-dimensional $SrRu_2O_6$, 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_2RuO_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_2RuO_4.

* This work was supported by the European Research Council under Advanced Grant No. 669550 (Com4Com).

1) H. Suzuki *et al.*, Nature Materials, 25 March (2019).
2) H. Gretarsson *et al.*, unpublished.
3) A. Jain *et al.*, Nature Physics **13**, 633 (2017).
4) G. Khaliullin, Phys. Rev. Lett. **111**, 197201 (2013).

Tuning the magnetocrystalline anisotropy in *R*CoPO by means of *R* substitution: a ferromagnetic resonance study

G. Prando[1], A. Alfonsov[2], A. Pal[3], V. P. S. Awana[3], B. Büchner[2], V. Kataev[2]

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

In *R*CoPO 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 *R*CoPO (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-*Tc* superconductors.

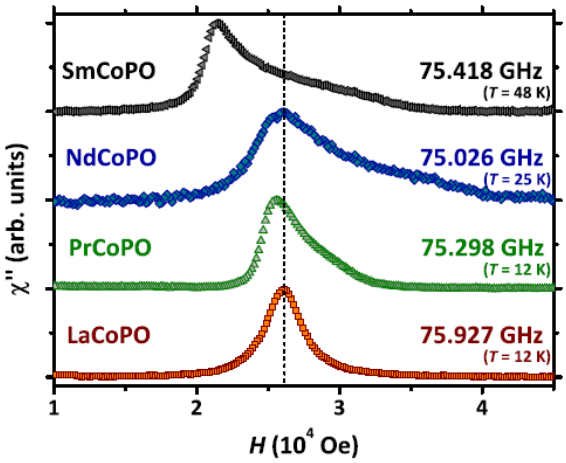


Figure: Experimental ferromagnetic resonance lines at comparable frequencies for the four investigated samples at different temperature values safely within the FM phase. The vertical dashed line denotes the central position for the resonance line of LaCoPO. Curves are shifted vertically for the aim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

1) G. Prando *et al.*, Phys. Rev. B **87**, 064401 (2013).
2) G. Prando *et al.*, Phys. Rev. B **92**, 144414 (2015).
3) G. Prando *et al.*, Phys. Rev. B **94**, 024412 (2016).

Electronic states of phonon Hall materials

Michiyasu Mori
Advanced Science Research Center, Japan Atomic Energy Agency, Tokai 317-1195, Japan

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, $Tb_3Ga_5O_{12}$ (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, $Ba_3CuSb_2O_9$ (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 contains 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.

1) C. Strohm, G. L. J. A. Rikken, and P. Wyder, Phys. Rev. Lett. **95**, 155901 (2005).
2) A. V. Inyushkin and A. N. Taldenkov, JETP Lett. **86**, 379 (2007).
3) Y. Hirogane, Y. Nii, Y. Tomioka, and Y. Onose, Phys. Rev. B **99**, 134419 (2019).
4) K. Sugii, M. Shimozawa, D. Watanabe, Y. Suzuki, M. Halim, M. Kimata, Y. Matsumoto, S. Nakatsuji, and M. Yamashita, Phys. Rev. Lett. **118**, 145902 (2017).
5) J. A. Quilliam, F. Bert, E. Kermarrec, C. Payen, C. Guillot-Deudon, P. Bonville, C. Baines, H. Luetkens, and P. Mendels, Phys. Rev. Lett. **109**, 117203 (2012).
6) M. Mori, A. Spencer-Smith, O. P. Sushkov, and S. Maekawa, Phys. Rev. Lett. **113**, 265901 (2014).

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

Yoshihiko Okamoto
Department of Applied Physics, Nagoya University, Nagoya 464-8603, Japan

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 Ta_4SiTe_4 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 Ta_4SiTe_4 and its substituted compounds show high thermoelectric performance at low temperature [1,2]. Thermoelectric power of Ta_4SiTe_4 whisker crystals, shown in Fig. 1, reaches S = –400 μV K^{-1} at 100-200 K, while maintaining low electrical resistivity of ρ ~ 2 mΩ cm. These S and ρ yield a roughly twice larger power factor ($P = S^2/\rho$) than that in Bi_2Te_3-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].

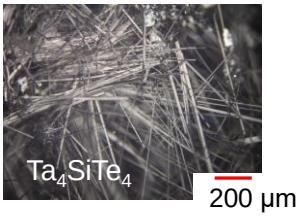


Fig. 1. Whisker crystals of Ta_4SiTe_4.

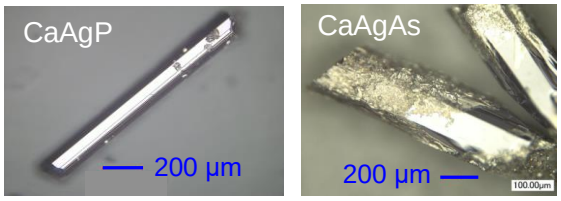


Fig. 2. Single crystals of CaAgP (left) and CaAgAs (right).

1) T. Inohara, Y. Okamoto, Y. Yamakawa, A. Yamakage, and K. Takenaka, Appl. Phys. Lett. **110**, 183901 (2017).
2) Y. Okamoto, T. Wada, Y. Yamakawa, T. Inohara, and K. Takenaka, Appl. Phys. Lett. **112**, 173905 (2018).
3) A. Yamakage, Y. Yamakawa, Y. Tanaka, and Y. Okamoto, J. Phys. Soc. Jpn. **85**, 013708 (2016).
4) Y. Okamoto, T. Inohara, A. Yamakage, Y. Yamakawa, and K. Takenaka, J. Phys. Soc. Jpn. **85**, 123701 (2016).

June 13 (Thu)

Poster Presentation

Gaussian-fluctuation Corrections to the phase diagram of *t-J* model

Masahiko Hayashi
Faculty of Education and Human Studies, Akita University, 1-1 Tegatagakuen-machi, 010-8502 Akita, Japan

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.

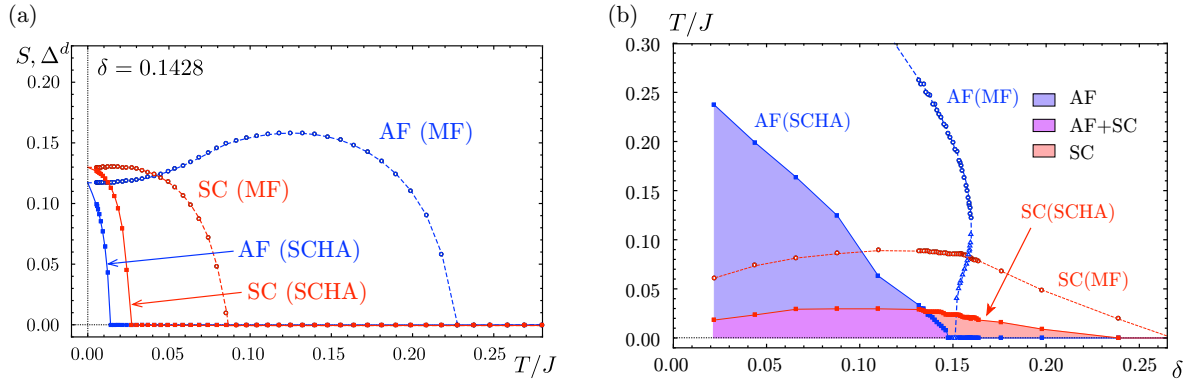


Figure 1: (a) Temperature T dependence of the AF and SC order parameters in the t-J model. Here, δ is the doping. (b) The fluctuation-corrected phase diagram of the t-J model. In each figure, MF and SCHA indicates the results of mean-field and self-consistent harmonic approximation. In (a), the transition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

1) M. Hayashi, Y. Tanuma, and K. Kuboki, J. Phys. Soc. Jpn. 82, 124705 (2013).

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

Hisatoshi Yokoyama[1], Ryo Sato[1], Kenji Kobayashi[2], Tsutomu Watanabe[2], and Masao Ogata[3]

[1] *Department of Physics, Tohoku University, Sendai 980-8578, Japan*

[2] *Department of Natural Science, Chiba Institute of Technology, Narashino 275-0023, Japan*

[3] *Department of Physics, University of Tokyo, Tokyo 113-0033, Japan*

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 concerts with local electron correlations. Recently, we found that the addition of a one-body projection factor $P(\theta)$ 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 $P(\theta)$ 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 $V = V_U^{(\pm)}$, with $|V_U| \sim U - |E_{\rm c}|$. Here, $E_{\rm c}$ ($\sim -t$) 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 $\delta_{\rm imp}$. (a) For $\delta_{\rm imp} < \delta$, the state is always metallic. (b) For $\delta_{\rm imp} = \delta$, the state becomes insulating for $V > V_{\rm M}$ ($\sim t$). (c) For $\delta_{\rm imp} > \delta$, the state becomes insulating for $V_{\rm M} < V < V_U^{(+)}$. We can intuitively interpret such behavior by virtue of Mott physics. We also would like to refer to large-$\delta_{\rm imp}$ cases.

* This study is partly supported by Grants-in-Aid from the Ministry of Education, Culture, Sports, Science and Technology, Japan.

[1] H. Yokoyama, R. Sato, and K. Kobayashi, J. Phys. Conf. Ser. **871**, 012032 (2017); *ibid.* **1054**, 012014 (2018).

[2] H. Yokoyama, R. Sato, and K. Kobayashi, to be published in J. Phys. Conf. Ser. (2019).

[3] R. Sato and H. Yokoyama, to be published in J. Phys. Conf. Ser. (2019).

[4] T. M. Rice and W. F. Brinkman, Phys. Rev. B **5**, 4350 (1972).

Self-Restraint Effect of Superconductivity due to Spin Fluctuations

Muhammad Zafur, Hiroyuki Yamase
Department of Condensed Matter Physics, Hokkaido University, Sapporo 060-0810, Japan
National Institute for Materials Science, Tsukuba 305-0047, Japan

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.

[1] I. I. Mazin, D. J. Singh, M. D. Johannes, and M. H. Du, Phys. Rev. Lett. **101**, 057003 (2008)
[2] K. Kuroki *et al*., Phys. Rev. Lett. **101**, 087004 (2008).
[3] T. Agatsuma and H. Yamase (unpublished).

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

Shun Asano[1, 2], Kenji Ishii[3], Daiju Matsumura[4], Takuya Tsuji[4], Toshiaki Ina[5], Kensuke M. Suzuki[2], and Masaki Fujita[2]

[1]*Department of Physics, Tohoku University, Sendai 980-8578, Japan*
[2]*Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan*
[3]*Synchrotron Radiation Research Center, National Institutes for Quantum and Radiological Science and Technology, Sayo 679-5148, Japan*
[4]*Materials Sciences Research Center, Japan Atomic Energy Agency, Sayo 679-5148, Japan*
[5]*Japan Synchrotron radiation Research Institute, Sayo 679-5148, Japan*

For the emergence of superconductivity in T'-type $RE_{2-x}Ce_xCuO_4$ (*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 [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 [4]. The evolution of the electronic states against oxygens variation (δ) at several x values in $Pr_{2-x}Ce_xCuO_{4+\alpha-\delta}$ (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 1*s*-4*pπ* dipole transition for Cu^+. 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 2δ suggests the emergence of not only electrons but also holes due to annealing.

1) D. Song *et al*., Phys. Rev. Lett. **118**, 137001 (2017).
2) M. Horio *et al*, Phys. Rev. Lett. **120**, 257001 (2018).
3) M. Horio *et al*., Phys. Rev. B **98**, 020505(R) (2018).
4) S. Asano *et al*., J. Phys. Soc. Jpn. **87**, 094710 (2018).

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

Makoto Mitarashi[1, 2], Terutoshi Sakakura[2], Hiroyuki Kimura[2], Shun Asano[1, 3], Kenji Tsutsumi[3], Masaki Fujita[3], Takuya Sumura[4], Tadashi Adachi[4], Yoji Koike[5], and Shunji Kishimoto[6]

[1]*Department of Physics, Tohoku University, Sendai 980-8578, Japan*

[2]*Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai 980-8577, Japan*

[3]*Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan*

[4]*Department of Engineering and Applied Sciences, Sophia University, Tokyo 102-8554, Japan*

[5]*Department of Applied Physics, Tohoku University, Sendai 980-8579, Japan*

[6]*Institute for Materials Structure Science, KEK, Tsukuba 305-0801, Japan*

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_2O_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 $Pr_{2-x}La_xCuO_{4+\delta}$, $Nd_2CuO_{4+\delta}$ and $Pr_{1.3-x}La_{0.7}Ce_xCuO_{4+\delta}$ (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_2O_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	dynamic reduced
O1 *occ.* (%)	101.7(7)	102.3(5)	99.2(2)
O2 *occ.* (%)	103.1(6)	102.4(5)	100.5(3)
Cu bond valence	1.7289(5)	1.7245(5)	1.7159(5)

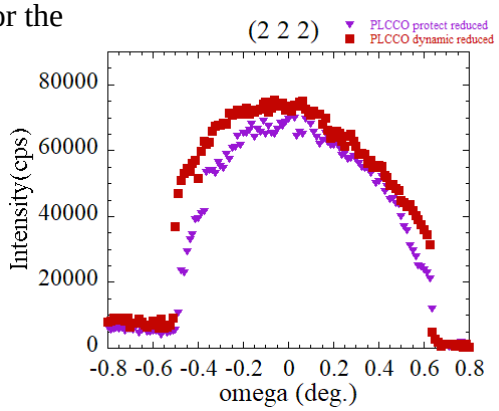


Figure 1 Bragg peak from the second phase

1) O. Matsumoto *et al.*, Physica C **469,** 924 (2009).
2) T. Adachi *et al.*, J. Phys. Soc. Jpn. **82,** 063713 (2013).
3) P. G. Radaelli *et al.*, Phys. Rev. B **49,** 15322 (1994).
4) H. Kimura *et al.*, J. Phys. Soc. Jpn. **74,** 2282 (2005).
5) H. J. Kang *et al.*, Nature Mat. **6,** 224 (2007).

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

Kohei Yamagami[1], Kenji Ishii[2], Yasuyuki Hirata[1], Keisuke Ikeda[1], Jun Miyawaki[1], Yoshihisa Harada[1], Shun Asano[3], Masaki Fujita[3], and Hiroki Wadati[4]

[1] *Institute for Solid State Physics, University of Tokyo, Kashiwa, Chiba 277-8581, Japan*

[2] *Synchrotron Radiation Research Center, National Institutes for Quantum and Radiological Science and Technology, Sayo, Hyogo 679-5148, Japan*

[3] *Institute for Materials Research, Tohoku University, Sendai, Miyagi 980-8577, Japan*

[4] *School of Science, University of Hyogo, Kamigori, Hyogo 678-1297, Japan*

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-T_c superconducting cuprate $La_{2-x}Sr_xCuO_4$ as well as its isostructural nickelate $La_{2-x}Sr_xNiO_4$.

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 chrage 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 $La_{2-x}Sr_xNiO_{4+\delta}$ with hole density ($n_h = x + 2\delta$) 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 La_2NiO_4 ($\sim$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 NiO_2 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].

1) J. Zaanen *et al.*, Phys. Rev. Lett. **55**, 418 (1985).
2) C. T. Chen *et al.*, Phys. Rev. Lett. **66**, 104 (1991).
3) E. Pellegrin *et al.*, Phys. Rev. B **53**, 10667 (1996).
4) K. Ishii *et al.*, Phys. Rev. B **96**, 115148 (2017).
5) T. Katsufuji *et al.*, Phys. Rev. B **54**, R14230 (1996).
6) K. Ishizaka *et al.*, Phys. Rev. B **67**, 184418 (2003).

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

S. Sugiura[1], T. Terashima[1], S. Yasuzuka[2], J. A. Schlueter[3], and S. Uji[1]
[1] *National Institute for Materials Science (NIMS), Tsukuba 305-0003, Japan*
[2] *Hiroshima Institute of Technology, Hiroshima 731-5193, Japan*
[3] *National Science Foundation, Virginia 22230, USA*

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 β"-$(ET)_2SF_5CH_2CF_2SO_3$ 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.

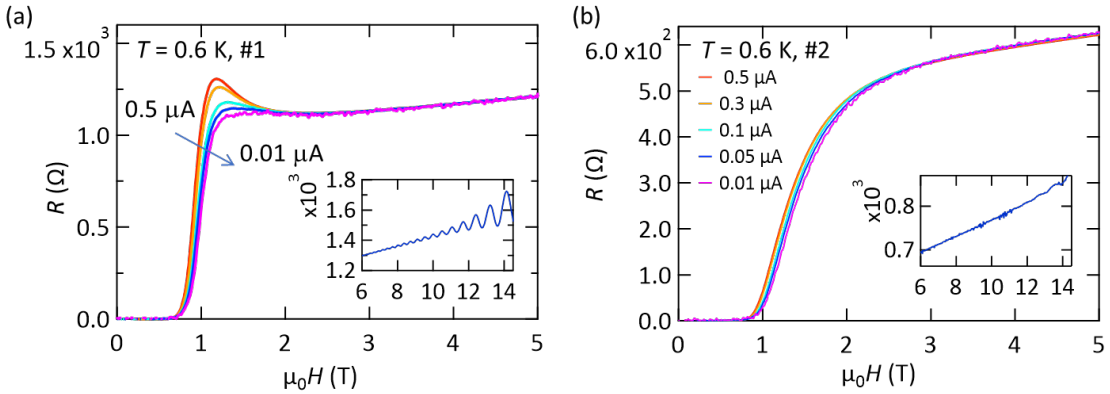


Figure 1: Magnetic field dependences of the interlayer resistance of (a) high-quality (#1) and (b) low-quality (#2) samples at 0.6 K for various current values, respectively. Insets show the Shubnikov-de Haas oscillations.

1) X. Su et al., *Phys. Rev. B* **59**, 6, 4376 (1999).
2) S. Uji et al., *Phys. Rev. B* **97**, 024505 (2018).
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

Takanori Taniguchi[1, 2], Shunsaku Kitagawa[1], Masahiro Manago[1],
Genki Nakamine[1], Kenji Ishida[1], and Hiroaki Shishido[3]
[1] *Department of Physics, Kyoto University, Kyoto 606-8502, Japan*
[2] *Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan*
[3] *Department of Physics and Electronics, Osaka Prefecture University, Osaka 980-8577, Japan*

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 $H_{c2} \sim 5$ (12) 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.

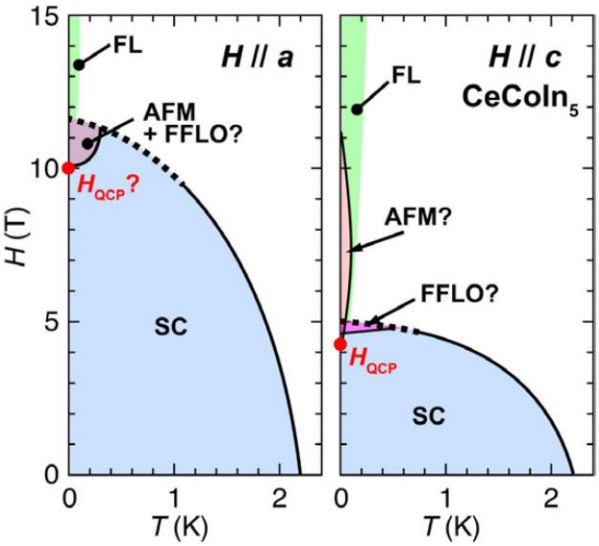


Figure 1: $H - T$ phase diagrams of $CeCoIn_5$ [3].

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 $1/T_1T$ 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 $1/T_1T$ near H_{c2}.

*This work was financially supported by JSPS/MEXT for Scientific Research (KAKENHI) Grant Numbers JP15H05882, JP15H05884, JP15H05745, JP17K14339, and JP19K03751. T. Taniguchi was supported by JSPS Research Fellowship (JP17J08806).

1) P. Fulde and R. A. Ferrell, Phys. Rev. 135, A550 (1964).
2) A. I. Larkin and Y. N. Ovchinnikov, Sov. Phys. JETP, 20, 762 (1965).
3) M. Shimozawa et al., Rep. Prog. Phys. 79, 074503 (2016).
4) H. Sakai et al, Phys. Rev. Lett. 107, 137001 (2011).
5) T. Tayama et al., Phys. Rev. B. 65, 180504(R).
6) K. Kumagai et al., J. Phys. Conf. Ser. 150, 052135 (2009).

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

Jan Fikáček[1], Jonas Warmuth[2], Fabian Arnold[3], Sunil Wilfred[4], Cinthia Piamonteze[5], Martin Bremholm[3], Jan Minár[4], Philip Hofmann[3], Jens Wiebe[2], and Jan Honolka[1]

[1]*Center for Analysis of Functional Materials, Institute of Physics of Czech Academy of Sciences, Na Slovance 1999/2, 182 21 Prague 8, Czech Republic*

[2]*Department of Physics, Hamburg University, Hamburg, Germany*

[3] *Department of Chemistry and Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), Aarhus University, 8000 Aarhus C, Denmark*

[4]*New Technologies Research Centre, University of West Bohemia, Plzeň, Czech Republic*

[5]*Paul Scherrer Institut, Forschungsstrasse 111, 5232 Villigen PSI, Switzerland*

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 $T_c = 8$ 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 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 $T_N \sim 70$K. In contrary, XMLD signals increase monotonically below T_N down to lowest temperatures ~ 2 K. XMLD data are compared with results of our density functional theory calculations.

*This work was supported by the German Science Foundation (DFG) via the DFG priority programme SPP1666 (grant no. WI 3097/2).

[1] F. C. Hsu et al., PNAS **105**, 14262 (2008).
[2] S. L. He et al, Nat. Mater. **12**, 605 (2013).
[3] J.-F. Ge et al., Nat. Mater. **14**, 285–289 (2015).
[4] X. Liu et al., J. Phys.: Cond. Mat. **27**, 183201 (2015).
[5] S. Manna et al., Nature Comm. **8**, 14074 (2017).

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

G. Prando[1], M. Moroni[1], E. Civardi[1], M. Babij[2], Z. Bukowski[2], S. Aswartham[3], I. Morozov[3,4], B. Büchner[3], H.-J. Grafe[3], P. Carretta[1]

[1]*Department of Physics, University of Pavia, Pavia, Italy*
[2]*Polish Academy of Sciences, Wrocław, Poland*
[3]*Leibniz-IFW Dresden, Dresden, Germany*
[4]*Lomonosov Moscow State University, Moscow, Russia*

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 3*d* 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 $RbFe_2As_2$ and $CsFe_2As_2$. 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 $T_0 \simeq$ 150 K and 75 K (for $RbFe_2As_2$ and $CsFe_2As_2$ respectively) and that eventually it splits into two distinct peaks for $RbFe_2As_2$ 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 $RbFe_2As_2$ 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.

1) E. Civardi *et al.*, Phys. Rev. Lett. **117**, 217001 (2016).
2) M. Moroni, G. Prando *et al.*, arXiv:1903.05029 (2019).

Influence of hydrostatic pressure and of Eu/Bi substitution on the magnetic properties of $Eu_2Ir_2O_7$

G. Prando[1], P. Telang[2], R. Dally[3], K. Mishra[2], W. Schottenhamel[4], Z. Guguchia[5], A. U. B. Wolter[4], A. K. Sood[6], S. D. Wilson[7], B. Büchner[4], M. J. Graf[3], S. Singh[2,8]

[1]*Department of Physics, University of Pavia, Pavia, Italy*
[2]*Department of Physics, IISER, Pune, India*
[3]*Department of Physics, Boston College, Chestnut Hill, Massachusetts, USA*
[4]*Leibniz-IFW Dresden, Dresden, Germany*
[5]*Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institut, Switzerland*
[6]*Department of Physics, Indian Institute of Sciences, Bangalore, India*
[7]*Department of Materials, University of California, Santa Barbara, California, USA*
[8]*Center for Energy Sciences, IISER, Pune, India*

The arrangement of magnetic moments at the vertices of a pyrochlore lattice leads to a great variety of electronic ground states for $R_2M_2O_7$ materials. One important finding common to several families of these oxides is that changes in r_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 r_I related to a gradual chemical substitution. Moreover, the metal-to-insulator transition in $R_2Ir_2O_7$ is associated with a dramatic change in the magnetic behavior as well.

Here, we report on the magnetic properties of $Eu_2Ir_2O_7$ under pressure, both from dc magnetometry and μ^+SR [1]. The absence of a localized magnetic moment from *f* shells in $Eu_2Ir_2O_7$ 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 μ+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 $(Eu_{1-x}Bi_x)_2Ir_2O_7$ 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 metalllic 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.

1) G. Prando *et al.*, Phys. Rev. B **93**, 104422 (2016).
2) P. Telang, K. Mishra, G. Prando, A. K. Sood, and S. Singh, arXiv:1902.03214 (2019).

June 14 (Fri)

Oral Presentation

Suppression of Antiferromagnetic Spin Fluctuations by Electron Doping in T'-$Pr_{1.3-x}La_{0.7}Ce_xCuO_4$ Probed by NMR

H. Fukazawa[1], YS. Lee[1], S. Kanamaru[1], M. Goto[1], Y. Kohori[1], A. Takahashi[2], T. Kawamata[2], K. Kawabata[3], K. Tajima[3], T. Adachi[3] and Y. Koike[2]

[1] *Dept. of Phys., Grad. Sch. of Sci., Chiba Univ., Chiba 263-8522, Japan*
[2] *Dept. of Appl. Phys., Grad. Sch. of Eng., Tohoku Univ., Sendai 980-8579, Japan*
[3] *Dept. of Eng. and Appl. Sci., Sophia Univ., Chiyoda, Tokyo 102-8554, Japan*

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'-$Pr_{1.3-x}La_{0.7}Ce_xCuO_4$ (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.

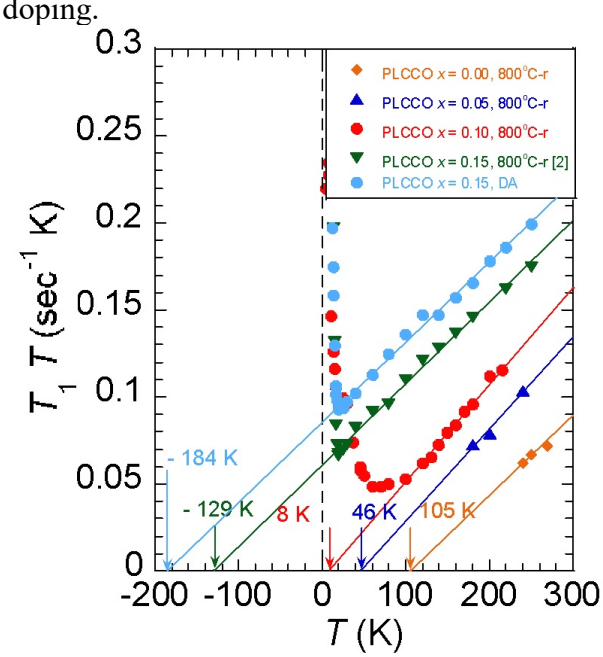


Figure 1: Temperature dependence of the spin-lattice relaxation time multiplied by temperature T_1T of the 800°C-reduced samples of T'-$Pr_{1.3-x}La_{0.7}Ce_xCuO_{4+\delta}$ (T'-PLCCO) (x = 0.00, 0.05, 0.10 and 0.15) and the dynamic-annealed T'-PLCCO (x = 0.15). Solid lines denote the fitted results of the Curie-Weiss-like fitting described in the text.

*This work was partially supported by JSPS KAKENHI Grant Numbers 16K05458, 17H02915 and 18K03505.

1) O. Matsumoto *et al.*, Physica C **469**, 924-927 (2009).
2) M. Yamamoto *et al*, J. Phys. Soc. Jpn. **85**, 024708 (2016).
3) T. Moriya, J. Magn. Magn. Mater. **100**, 261 (1991).

Electron doping in the undoped (Ce-free) superconductor T'-$La_{1.8}Eu_{0.2}CuO_4$

T. Kawamata, T. Sunohara, K. Shiosaka, T. Takamatsu, T. Noji, M. Kato, and Y. Koike
Department of Applied Physics, Tohoku University, Sendai 980-8579, Japan

The superconductivity in undoped (Ce-free) Ln_2CuO_4 (*Ln*: lanthanide elements) with the Nd_2CuO_4-type (so-called T'-type) structure emerges via the adequate reduction annealing without the substitution of Ce for *Ln*, namely, without extra electron doping [1-2]. In the polycrystalline bulk sample of T'-$La_{1.8}Eu_{0.2}CuO_4$, 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'-$La_{1.8-x}Eu_{0.2}M_xCuO_4$ (*M* = Sr, 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'-$La_{1.8}Eu_{0.2}CuO_4$ by the Ce substitution to La.

Here, we have succeeded in synthesizing the electron-doped polycrystalline bulk samples of T'-$La_{1.8}Eu_{0.2}CuO_{4-y}F_y$ (y = 0-0.15) by the fluorination of T'-$La_{1.8}Eu_{0.2}CuO_4$ using NH_4F. The magnetic susceptibility measurements have revealed that T_c increases with increasing y, exhibits the maximum of ~23 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].

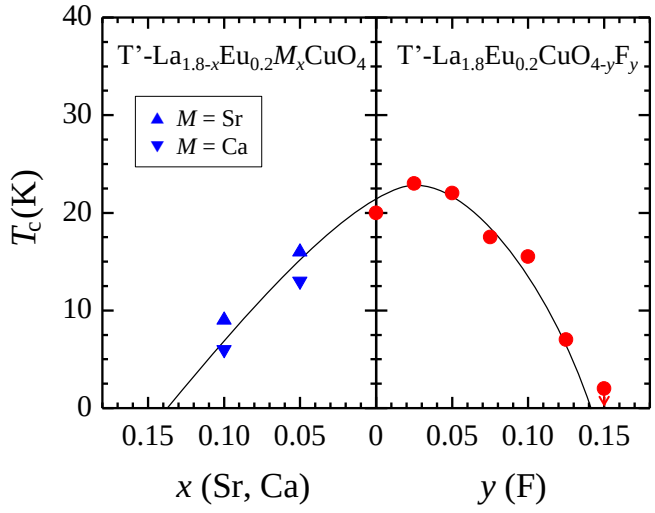


Figure 1: Carrier-concentration dependence of critical temperature, T_c, for T'-$La_{1.8-x}Eu_{0.2}M_xCuO_4$ (*M* = Sr, Ca)[3,4] and T'-$La_{1.8}Eu_{0.2}CuO_{4-y}F_y$. Solid lines are guides to eyes.

*This work was partially supported by JSPS KAKENHI Grant Numbers 17H02915.

1) O. Matsumoto *et al.*, Physica C **469**, 924 (2009).
2) O. Matsumoto *et al.*, Phys. Rev. B **79**, 100508(R) (2009).
3) T. Takamatsu *et al.*, Phys. Express **5**, 073101 (2012).
4) T. Takamatsu *et al.*, Physics Procedia **58**, 46 (2014).
5) K. Yamazaki *et al.*, J. Phys: Conf. Ser. **871**, 012009 (2017).

Engineering the Mott State of Cuprates for High-Temperature Superconductivity

O. Ivashko[1], M. Horio[1], W. Wan[2], N. B. Christensen[2], D. E. McNally[3], E. Paris[3], Y. Tseng[3], N. E. Shaik[4], H. M. Rønnow[4], H. I. Wei[5], C. Adamo[6], C. Lichtensteiger[7], M. Gibert[1], M. R. Beasley[6], K. M. Shen[5], J. M. Tomczak[8], T. Schmitt[3], J. Chang[1]

[1]*Physik-Institut, Universität Zürich, Winterthurerstrasse 190, CH-8057 Zurich, Switzerland*
[2]*Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark*
[3]*Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland*
[4]*Institute of Physics, Ecole Polytechnique Federale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland*
[5]*Department of Physics, Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York 14853, USA*
[6]*Department of Applied Physics, Stanford University, Stanford, CA 94305, USA*
[7]*Department of Quantum Matter Physics, University of Geneva, 24 Quai Ernest Ansermet, 1211 Geneva, Switzerland*
[8]*Institute of Solid State Physics, Vienna University of Technology, A-1040 Vienna, Austria*

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 $La_{2-x}Sr_xCuO_4$ (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 La_2CuO_4 films can be tuned through strain [4]. We noticed that films with the largest exchange interaction also has the highest superconducting transition T_c upon doping – consistent with a magnetic pairing scenario.

References

[1] C.E. Matt *et al*., Nat. Comm. **9**, 972 (2018)
[2] M. Horio *et al*., Nat. Comm. **9**, 3252 (2018)
[3] M. Horio *et al*., PRL **121**, 77004 (2018)
[4] O. Ivashko *et al*., Nat. Comm. **10**, 786 (2019)

Superconductivity drives magnetism in δ-doped La_2CuO_4

A. Suter[1], G. Logvenov[2], A.V. Boris[2], F. Baiutti[2], F. Wrobel[2], L. Howald[3], E. Stilp[4], Z. Salman[1], T. Prokscha[1], and B. Keimer[2]

[1] *Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland*

[2] *Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany*

[3] *SLS, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland*

[4] *Materials for Energy Conversion, Empa, CH-8600 Dübendorf, Switzerland*

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 δ-doped La_2CuO_4 (δ-LCO_N) superlattices. By means of molecular beam epitaxy whole 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 μSR. 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.

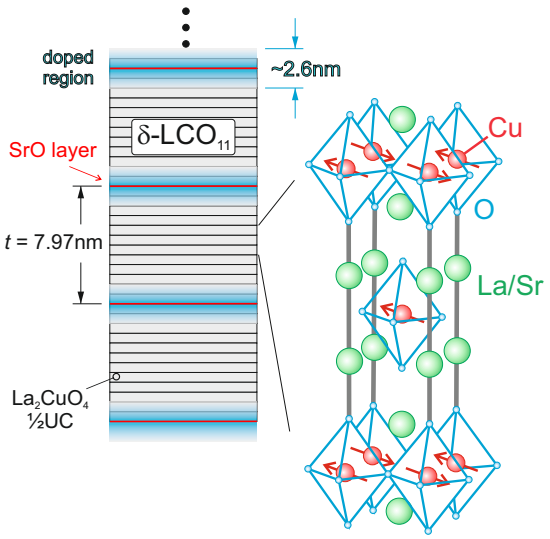


Figure 1: Sketch of delta doped La_2CuO_4 for $N = 11$. Starting from La_2CuO_4, a superlattice is formed by replacing single layers of LaO with SrO planes.

Uniaxial pressure control of competing orders in the cuprates

H.-H. Kim[1], S. M. Souliou[2], M.E. Barber[3], E. Lefrancois[1,2], M. Minola[1], R. Heid[4], A. Bosak[2], A. P. Mackenzie[3], B. Keimer[1], C. W. Hicks[3], M. Le Tacon[4]

[1]Max Planck Institute for Solid State Research, Stuttgart, Germany.
[2]European Synchrotron Radiation Facility (ESRF), Grenoble, France.
[3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany.
[4]Institute for Solid State Physics, Karlsruhe Institute of Technology, Karlsruhe, Germany.

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 YBa2Cu3O6.67 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 an illustrate the potential of uniaxial-pressure control of competing orders in quantum materials [1].

1) H.-H. Kim, S. M. Souliou et al., *Science* **362**, 1040 (2018).

Probing CDW phenomena and charge excitations in cuprates via RIXS

Wei-Sheng Lee
Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Lab.

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].

*This work supported by the Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract DE-AC02-76SF00515.

1) L. Chaix et al., Dispersive charge density wave excitations in underdoped cuprates Bi2Sr2CaCu2O8+d. Nature Physics 13, 952 (2017).
2) H. Lu *et al*., in preparation.
3) M. Hepting *et al*., Three-dimensional collective charge excitations in electron-doped copper oxide superconductors. Nature 563, 374 (2018).

Dual structure in the charge excitation spectrum of electron-doped cuprates

Matías Bejas[1], Hiroyuki Yamase[2], and Andrés Greco[1]
[1] *Facultad de Ciencias Exactas, Ingeniería y Agrimensura and Instituto de Física Rosario (UNR-CONICET), Avenida Pellegrini 250, 2000 Rosario, Argentina*
[2] *National Institute for Materials Science, Tsukuba 305-0047, Japan*

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].

1) E. H. da Silva Neto *et al.*, Science **347**, 282 (2015).
2) E. H. da Silva Neto *et al.*, Sci. Adv. **2**, 1600782 (2016).
3) W. S. Lee *et al.*, Nat. Phys. **10**, 883 (2014).
4) K. Ishii *et al.*, Nat. Commun. **5**, 3714 (2014).
5) M. Hepting *et al.*, Nature **563**, 374378 (2018).
6) M. Bejas, H. Yamase, and A. Greco, Phys. Rev. B **96**, 214513 (2017).
7) H. Yamase, M. Bejas, and A. Greco EPL, **111** 57005 (2015).
8) H. Yamase, M. Bejas, and A. Greco, Phys. Rev. B **99**, 014513 (2019).
9) A. Greco, H. Yamase, and M. Bejas, Phys. Rev. B **94**, 075139 (2016).
10) A. Greco, H. Yamase, and M. Bejas, Commun.Phys. **2**, 3 (2019).

Three-dimensional Fermi surface of overdoped La-based cuprates

M. Horio[1], K. Hauser[1], Y. Sassa[2], Z. Mingazheva[1], D. Sutter[1], K. Kramer[1], A. Cook[1], E. Nocerino[3], O. K. Forslund[3], O. Tjernberg[3], M. Kobayashi[4], A. Chikina[4], N. B. M. Schröter[4], J. A. Krieger[5,6], T. Schmitt[4], V. N. Strocov[4], S. Pyon[7], T. Takayama[7], H. Takagi[7], O. J. Lipscombe[8], S. M. Hayden[8], M. Ishikado[9], H. Eisaki[10], T. Neupert[10], M. Månsson[3], C. E. Matt[1,4,11], and J. Chang[1]

[1]*Physik-Institut, Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland*
[2]*Department of Physics and Astronomy, Uppsala University, SE-75121 Uppsala, Sweden*
[3]*Department of Applied Physics, KTH Royal Institute of Technology, Electrum 229, SE-16440 Stockholm Kista, Sweden*
[4]*Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland*
[5]*Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland*
[6]*Laboratorium für Festkörperphysik, ETH Zürich, CH-8093 Zürich, Switzerland*
[7]*Department of Advanced Materials, University of Tokyo, Kashiwa 277-8561, Japan*
[8]*H. H. Wills Physics Laboratory, University of Bristol, Bristol BS8 1TL, United Kingdom*
[9]*Comprehensive Research Organization for Science and Society (CROSS), Tokai, Ibaraki 319-1106, Japan*
[10]*Electronics and Photonics Research Institute, National Institute of Advanced Industrial Science and Technology, Ibaraki 305-8568, Japan*
[11]*Department of Physics, Harvard University, Cambridge, MA 02138, USA*

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 $La_{2-x}Sr_xCuO_4$ and $Eu_{0.2}La_{1.8-x}Sr_xCuO_4$, 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.

*This work supported by the Swiss National Science Foundation.

[1] N. Doiron-Leyraud *et al*., Nat. Commun. **8**, 2044 (2017).
[2] W. Wu *et al*., Phys. Rev. X **8**, 021048 (2018).
[3] N. Momono *et al*., Physica C **233**, 395 (1994).
[4] B. Michon *et al*., Nature **567**, 218 (2019).
[5] M. Horio *et al*., Phys. Rev. Lett. **121**, 077004 (2018).

π-tons – generic optical excitations of correlated systems

Anna Kauch, Petra Pudleiner, Katharina Astleithner, Tin Ribic, and Karsten Held
Institute of Solid State Physics, TU Wien, Vienna, Austria

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 $\mathbf{k} = (\pi, \pi, \ldots)$ or close to it, we called the derived polaritons π-tons. These π-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 (DΓA) and parquet approximations, implemented within the *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.

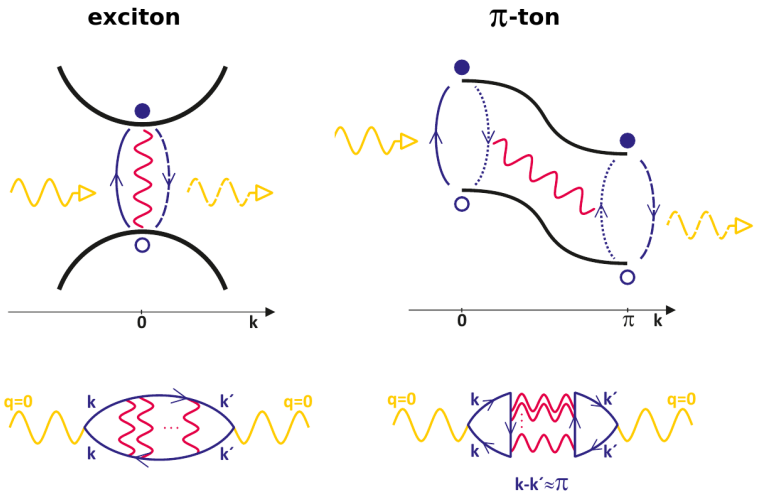


Figure 1: Sketch of the physical processes (top) and Feynman diagrams (bottom) behind an exciton (left) and a π-ton (right). The yellow line symbolizes the incoming (and outgoing) photon which creates an electron-hole pair denoted by open and filled circles, respectively. The Coulomb interaction between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

[1] A. Kauch, P. Pudleiner, K. Astleithner, T. Ribic, and K. Held, arXiv:1902.09342 (2019).
[2] G. Li, A. Kauch, P. Pudleiner, and K. Held, arXiv:1708.07457 (Comp. Phys. Comm. 2019).

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

Kazuhiro Kuboki[1]
[1] *Department of Physics, Kobe University, Kobe 657-8501, Japan*

Spatial distributions of spontaneous magnetic fields, **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 **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 **B** exists only in the region within the superconducting coherence length ξ_d from the surface. Outside the surface, magnetic fileds decay quickly, and the typical length scale for the decay is of the order of c_1, the distance between bilayer (a few $\mathring{A}$).

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 μSR or polarized neutron scattering.

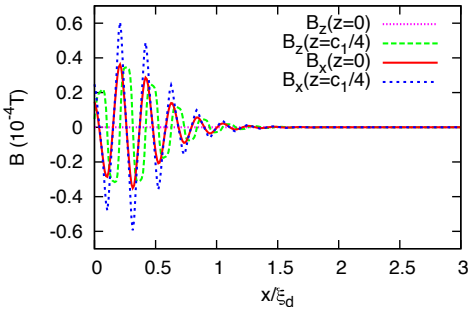


Figure 1: Spatial variations of B_z and B_x. $z=0$ corresponds to the center of a bilayer, and c_1 is the distance between two layers.

1) K. Kuboki, J. Phys. Soc. Jpn. **84**, 064706 (2015).
2) K. Kuboki, J. Phys. Soc. Jpn. **87**, 024703 (2018).
2) K. Kuboki, arXiv:1904.07474.

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

Suguru Nakata[1], Keisuke Koshiishi[1], Liang Liu[1], Atsushi Fujimori[1,2], Hiroshi Eisaki[3], and Shin-ichi Uchida[1,3]

[1]*Department of Physics, University of Tokyo, Tokyo 113-0033, Japan*
[2]*Department of Applied Physics, Waseda University, Tokyo 169-8555, Japan*
[3]*National Institute of Advanced Industrial Science and Technology, Tsukuba 305-8560, Japan*

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 $BaFe_2As_2$ [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].

This work has been done in collaboration with M. Horio, C. Lin, K. Okazaki, J. Xu, H. Suzuki , T. Shimojima, T. Yoshida, K. Kihou, C.-H. Lee, T. Ito, Y. Tomioka, A. Iyo, D. Song, Y. Yoshida, H. Kumigashira, M. Kobayashi, M. Minohara, K. Horiba, S. Ideta, and K. Tanaka. Discussion with H. Aoki, H. Kontani, T. Shibauchi, Y. Matsuda, and H. Yamase is gratefully acknowledged.

1) B. Keimer, S. A. Kivelson, M. R. Norman, S. Uchida, and J. Zaanen, Nature **518**, 179 (2015).
2) Y. Sato *et al.*, Nat. Phys. **13**, 1074 (2017); H. Maruyama *et al*., arXiv:1805.00276; O. Cyr-Choinière *et al.*, Phys. Rev. B **92**, 224502 (2015).
3) S. Nakata *et al.*, arXiv:1811.10028.
4) W.-L. Tu and T.-K. Lee, Sci. Rep. **9**, 1719 (2019).
5) S. Kasahara *et al.*, Nature **486**, 382 (2012).
6) M. Yi *et al.*, PNAS **108**, 6878 (2011); L. Liu *et al.*, Phys. Rev. B **92**, 094503 (2015); arXiv:1503.02855.
7) K. Koshiishi, Thesis (University of Tokyo, 2019).

Nematic fluctuation and resonance in $BaFe_2(As,P)_2$ observed by Raman scattering spectroscopy

S. Miyasaka[1], T. Adachi[1], M. Nakajima[1], and S. Tajima[1]
[1] *Department of Physics, Osaka University, Osaka 560-0043, Japan*

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.

1) J.-H. Chu *et al.* Science **329**, 824 (2010).
2) M. Yi *et al.*, PNAS **108**, 6878 (2011).
3) S. Kasahara *et al*., Nature **486**, 382 (2012).
4) Y. Gallais *et al*., Phys. Rev. Lett. **111**, 267001 (2013).
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

Seiichiro Onari and Hiroshi Kontani
Department of Physics, Nagoya University, Furo-cho, Nagoya 464-8602, Japan

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° from the conventional B_{1g} nematicity, has been discovered in heavily hole-doped ($n_d = 5.5$) compound AFe_2As_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_2As_2.

In $BaFe_2As_2$, 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.

1) S. Onari and H. Kontani, Phys. Rev. Lett. **109**, 137001 (2012).
2) J. Li *et al.*, arXiv:1611.04694.
3) X. Liu *et al.*, arXiv:1803.07304.
4) K. Ishida *et al.*, arXiv:1812.05267.
5) S. Onari, Y. Yamakawa, and H. Kontani, Phys. Rev. Lett. **116**, 227001 (2016).
6) S. Onari and H. Kontani, arXiv:1809.08017.
7) S. Kasahara *et al.*, Nature **486**, 382 (2012).
8) T. Shimojima *et al.*, Phys. Rev. B **89**, 045101 (2014).

Infrared Spectroscopic Studies of the Phonon Dynamics in Iron-based Superconductors

X.G. Qiu, R. Yang, B. Xu

National Laboratory for Superconductivity, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

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 $CaKFe_4As_4$

W.-L. Zhang [1,†], W. R. Meier [2,3], T. Kong [2,3], P. C. Canfield [2,3], and G. Blumberg [1,4]

[1] *Department of Physics & Astronomy, Rutgers University, Piscataway, New Jersey 08854,* USA
[2] *Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA*
[3] *Division of Materials Science and Engineering, Ames Laboratory, Ames, Iowa 50011, USA*
[4] *National Institute of Chemical Physics and Biophysics, Akadeemia tee 23, 12618 Tallinn, Estonia*
[†] *Present address: Department of Engineering and Applied Sciences, Sophia University, Tokyo 102-8554, Japan.*

Understanding the pairing mechanism in the Fe-based superconductors (FeSCs) remains in a focus of research not only due to a high superconducting transition temperature Tc, 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 Tc.

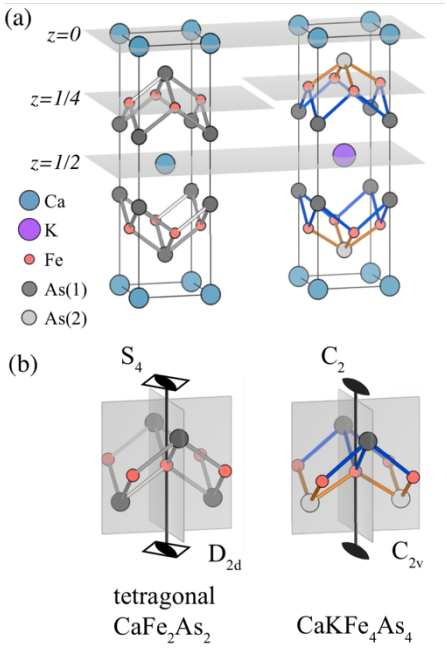


Figure 1: Comparison of (a) lattice structure and (b) Fe site symmetry in $CaFe_2As_2$ and $CaKFe_4As_4$.

A new class of stoichiometric and strictly tetragonal superconductors $CaAFe_4As_4$ (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 $CaKFe_4As_4$ 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 λ^{Γ}= 0.0015, which is very small for a superconductor with T_C at 35 K [1].

This work supported by the NSF Grant No. DMR-1709161, USDOE-BES under Contract No. DE-AC02-07CH11358, and Gordon and Betty Moore Foundation's EPiQS Initiative through Grant No. GBMF4411.

1) W.-L.Zhang *et al.*, Phys.Rev.B **98**, 140501 (2018)

Time-reversal symmetry breaking in the nematic superconductor FeSe

Takasada Shibauchi[1]
[1]*Department of Advanced Materials Science, University of Tokyo, Kashiwa 277-8561, Japan*

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 (μSR) 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.

1) T. Watashige *et al.*, Phys. Rev. X **5**, 031022 (2015).
2) T. Hashimoto *et al.*, Nat. Commun. **9**, 282 (2018).

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

Tadashi Machida[1], Yue Sun[2], Sunseng Pyon[3], Shun Takeda[4], Yuhki Kohsaka[1], Tetsuo Hanaguri[1], Takao Sasagawa[4] and Tsuyoshi Tamegai[3]

[1]*RIKEN Center for Emergent Matter Science (CEMS), Wako 351-0198, Japan*
[2]*Department of Physics and Mathematics, Aoyama Gakuin University Sagamihara, Kanagawa 252-5258, Japan*
[3]*Department of Applied Physics, University of Tokyo, Hongo, Tokyo 113-8656, Japan*
[4]*Laboratory for Materials and Structures, Tokyo Institute of Technology, Yokohama, Kanagawa 226-8503, Japan*

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 $FeTe_{0.6}Se_{0.4}$ with unprecedentedly high energy resolution of ~20 μeV. We found that a certain number of vortices possess the ZVBS below 20 μeV, 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.

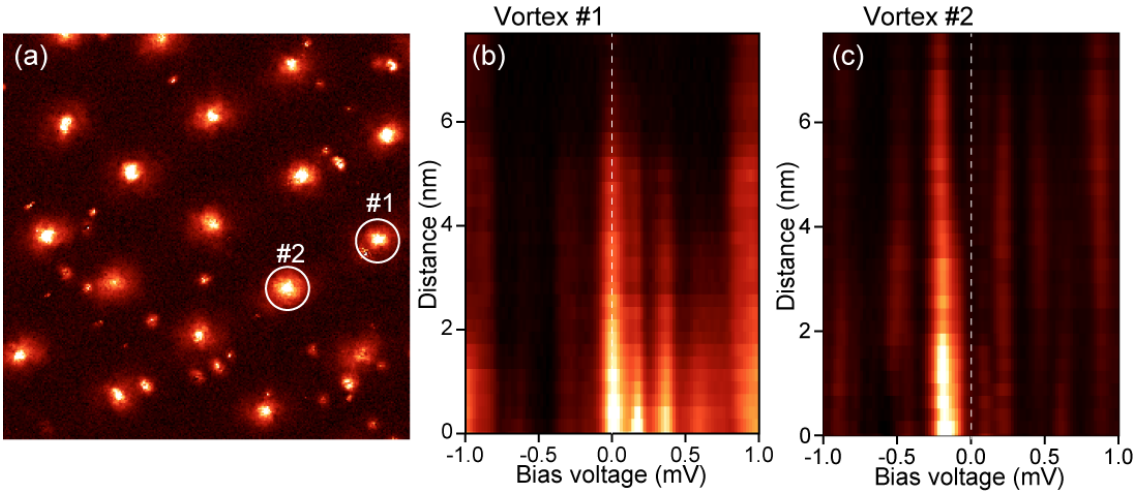


Figure 1. (a) A zero bias conductance map in a 187 nm x 187 nm field of view of a set point at V = -10 mV and I = 100 pA. (b) and (c) Line profiles of high energy resolution tunneling spectra across the vortex core with and without the ZVBS, respectively.

References

1) D. Wang *et al.*, Science **362**,333 (2018)
2) J. –P. Xu *et al.*, Phys. Rev. Lett. **114**, 017001 (2015)
3) Q. Liu *et al.*, Phy. Rev. X **8**, 041056 (2018)
4) M. Chen *et al.*, Nature Commun. **9**, 970 (2018)
5) T. Machida *et al.*, Rev. Sci. Instrum. **89**, 093707 (2018)
6) T. Machida *et al.*, arXiv.1812.08995 (2018)

Topological Ultranodal pair states in iron superconductors

Chandan Setty*, Shinibali Bhattacharyya*, Andreas Kreisel** and Peter J. Hirschfeld*
*University of Florida, Gainesville, FL, USA
** Institut fur Theoretische Physik Universitat Leipzig D-04103 Leipzig, Germany

We show that multiband superconductors with dominant spin singlet, intraband pairing of spin-1/2 electrons can undergo a transition to a state with Bogolibuov 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 FeSe1−xSx across the nematic transition, where this ``ultranodal'' 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

Xingjiang ZHOU

Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China
Email: XJZhou@iphy.ac.cn

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 (Tc). The origin of the dramatic Tc 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-Tc superconductivity. They also provide a new route of realizing superconductivity in iron based superconductors which is similar to that in high temperature cuprate superconductors.

*Work done in collaboration with Yong Hu, Yu Xu, Yi-Min Zhang, Qing-Yan Wang, Shao-Long He, De-Fa Liu, Ai-Ji Liang, Jian-Wei Huang, Cong Li, Yong-Qing Cai, Ding-Song Wu, Guo-Dong Liu, Fang-Sen Li, Jia-Qi Fan, Guan-Yu Zhou, Lili Wang, Can-Li Song, Xu-Cun Ma, Qi-Kun Xue, Zu-Yan Xu and Lin Zhao.

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

Kosue Nakayama

Department of Physics, Tohoku University, Sendai 980-8578, Japan

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 monoalyer 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.

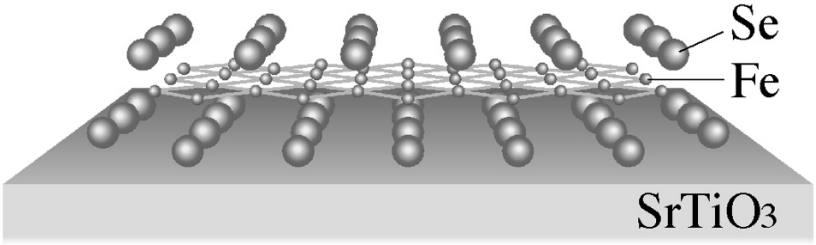


Figure 1: Schematic view of monolayer FeSe film on $SrTiO_3$ substrate.

1) Q.-Y. Wang *et al*., Chin. Phys. Lett. **29**, 037402 (2012).
2) S. He *et al*., Nat. Mater. **12**, 605 (2013).
3) S. Tan *et al*., Nat. Mater. **12**, 634 (2013).
4) Y. Miyata *et al*., Nat. Mater. **14**, 775 (2015).
5) J. J. Lee *et al*., Nature **515**, 245 (2014).

Comparison between Te- and S-substitution effects on superconductivity in FeSe thin films

Fuyuki Nabeshima[1], Tomoya Ishikawa[1], Naoki Shikama[1], Souta Nakamura[1], Hodaka Kurokawa[1], and Atsutaka Maeda[1]

[1] *Dept. of Basic Science, the University of Tokyo, Tokyo 153-8902, Japan*

We grew single crystalline films of $FeSe_{1-x}S_x$ with $x \leq 0.43$ 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 $FeSe_{1-x}S_x$ is similar to that of bulk $FeSe_{1-x}S_x$ except for the possible magnetic transition, but is in contrast to that of $FeSe_{1-y}Te_y$ films, which shows a sudden increase of T_c at the composition where the structural transition disappears[1)]. These results suggest that the nematicity has no universal significance on the superconductivity in FeSe[2)]. 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.

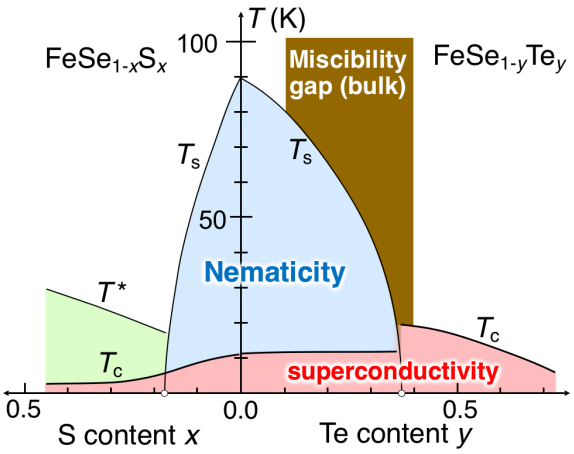


Figure 1: Schematic phase diagram of S- and Te-substituted FeSe thin films. T^* represents possible magnetic transition temperature.

1) Y. Imai *et al.*, Sci. Rep. 7, 46653 (2017).
2) F. Nabeshima *et al.*, J. Phys. Soc. Jpn. 87, 073704 (2018).

Ultrafast nematic-orbital excitation in FeSe

T. Shimojima[1,2], Y. Suzuki[2], A. Nakamura[1,2], N. Mitsuishi[2], S. Kasahara[3], T. Shibauchi[4], Y. Matsuda[3], Y. Ishida[5], S. Shin[5] and K. Ishizaka[1,2]

[1]RIKEN Center for Emergent Matter Science (CEMS), Wako 351-0198, Japan
[2]Quantum-Phase Electronics Center (QPEC) and Department of Applied Physics, The University of Tokyo, Tokyo 113-8656, Japan
[3]Department of Physics, Kyoto University, Kyoto 606-8502, Japan
[4]Department of Advanced Materials Science, The University of Tokyo, Kashiwa, 277-8561, Japan
[5]Institute for Solid State Physics (ISSP), The University of Tokyo, Kashiwa, 277-8581, Japan.

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 $3d_{xz}$ 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.

1) E. Fradkin *et al*., Annu. Rev. Condens. Matter Phys. **1**, 153-178 (2010).
2) R. M. Fernandes, A. V. Chubukov and J. Schmalian, Nat. Phys. **10**, 97-104 (2014).
3) Y. Sato *et al*., Nat. Phys. **13**, 1074-1078 (2017).
4) T. Shimojima *et al*., Phys. Rev. B **90**, 121111(R) (2014).
5) T. Shimojima *et al*., Nat. Commun. Accepted.

Dynamical magnetism in iron-based ladder compounds

Yusuke Nambu[1]
[1] *Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan*

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_2X_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 $BaFe_2S_3$ 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 $BaFe_2Se_3$ 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 $BaFe_2Se_3$ 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.

The research project was conducted through a collaboration with K.M. Suzuki, T. Hawai, M. Nagao, S. Itoh, H. Okabe, A. Koda, R. Kadono, S. Imaizumi, K. Hashizume, T. Aoyama, and K. Ohgushi.

1) Y. Nambu *et al.*, Phys. Rev. B **85**, 064413 (2012).
2) F. Du *et al.*, Phys. Rev. B **85**, 214436 (2012).
3) H. Takahashi *et al.*, Nat. Mat. **14**, 1008 (2015).

Exploration of Novel Pt-based Superconductors with Honeycomb Networks

Kazutaka Kudo
Research Institute for Interdisciplinary Science, Okayama University, Okayama 700-8530, Japan

Alkaline-earth platinum pnictides exhibit a variety of hexagonal structures that are characterized by honeycomb networks, such as $CaPt_xP_{2-x}$, 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 ($P\text{-}6m2$, 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- ($P\text{-}6m2$, 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).

1) Y. Nishikubo, K. Kudo, and M. Nohara, J. Phys. Soc. Jpn. **80**, 055002 (2011).
2) J. Goryo, M. H. Fischer, and M. Sigrist, Phys. Rev. B **86**, 100507(R) (2012).
3) M. H. Fischer, T. Neupert, C. Platt, A. P. Schnyder, W. Hanke, J. Goryo, R. Thomale, and M. Sigrist, Phys. Rev. B **89**, 020509(R) (2014).
4) W.-S. Wang, Y. Yang, and Q.-H. Wang, Phys. Rev. B **90**, 094514 (2014).
5) K. Kudo, Y. Saito, T. Takeuchi, S. Ayukawa, T. Kawamata, S. Nakamura, Y. Koike, and M. Nohara, J. Phys. Soc. Jpn. **87**, 063702 (2018).
6) T. Adachi, T. Sumura, K. Kawabata, S. Onishi, Y. Saito, K. Kudo, M. Nohara, I. Watanabe, A. Koda, H. Okabe, R. Kadono, and W. Higemoto, KEK-MSL Report 2017, 54 (2018).
7) K. Kudo, T. Takeuchi, H. Ota, Y. Saito, S. Ayukawa, K. Fujimura, and M. Nohara, J. Phys. Soc. Jpn. **87**, 073708 (2018).

Observation and control of nematic superconductivity in doped Bi_2Se_3 topological superconductors

Shingo Yonezawa[1]
[1]*Department of Physics, Graduate School of Science, Kyoto University*
Kyoto 606-8502, Japan

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 $A_xBi_2Se_3$ (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).

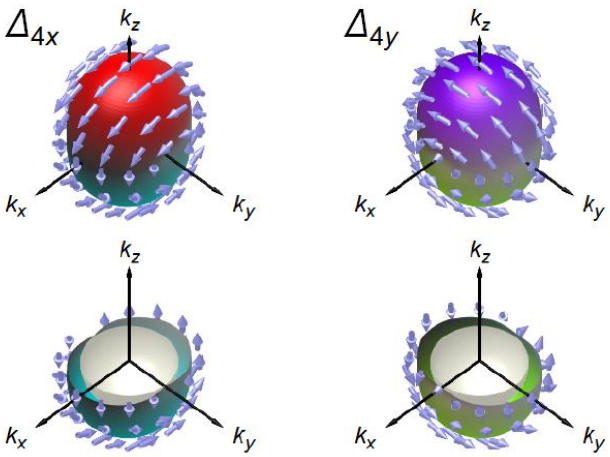


Figure 1: Schematic figures of the proposed gap structures for the nematic superconducting states in $A_xBi_2Se_3$, with horizontal cuts in the bottom row [1]. The arrows depict the *d*-vector order parameters; and the distance between the colored surface and the gray sphere explains the gap amplitude.

1) For a recent review, see S. Yonezawa, Condens. Matter **4**, 2 (2019).
2) K. Matano *et al.*, Nature Phys. **12**, 852 (2016).
3) S. Yonezawa *et al.*, Nature Phys. **13**, 123 (2017).
4) Y. Pan *et al.*, Sci. Rep. **6**, 28632 (2016).
5) R. Tao *et al.*, Phys. Rev. X **8**, 041024 (2018).

Effect of Antisymmetric Spin-Orbit Interaction on Critical Field of Ion-Gated 2D Superconductors

Tsutomu Nojima
Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

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 $4.3T_c$ for $SrTiO_3$-EDLT and $8T_c$ in MoS_2-EDLT [3] at low temperature, which exceed far the usual Pauli-Clogston-Chandrasekhar (paramagnetic depairing) limit of $1.8T_c$. 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).

[1] Y. Saito, T. Nojima, Y. Iwasa, Nat. Rev. Mater. 2, 16094 (2017).
[2] K. Ueno *et al*., Phys. Rev. B 89, 020508(R) (2014).
[3] Y. Saito *et al*., Nature Phys. 12, 144 (2016).
[4] Y. Nakamura and Y. Yanase, J. Phys. Soc. Jpn. 82, 083705 (2013).

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

S. Uji[1], S. Sugiura[1], T.Isono[1], N. Kikugawa[1], T. Terashima[1],
H. Akutsu[2], Y. Nakazawa[2], D. Graf[3], P. Day[4]
[1] *National Institute for Materials Science, Tsukuba 305-0003, Japan*
[2]*Osaka University, Toyonaka, Osaka 560-0043, Japan*
[3]*National High Magnetic Field Laboratory, Tallahassee, Florida 32310, USA*
[4]*University College London, London, United Kingdom*

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_{Pauli}. Layered organic superconductors are best candidates for the FFLO phase studies. In the FFLO phase, the order parameter is given by $\Delta(r) = \Delta_0\cos(\boldsymbol{qr})$, where $\boldsymbol{q}$ 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 $\lambda_{\mathrm{FFLO}} = 2\pi/q$ 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 ~ H_{Pauli} at low temperatures. On reasonable assumptions, we can estimate λ_{FFLO}, which decreases as the field approaches H_{c2}.

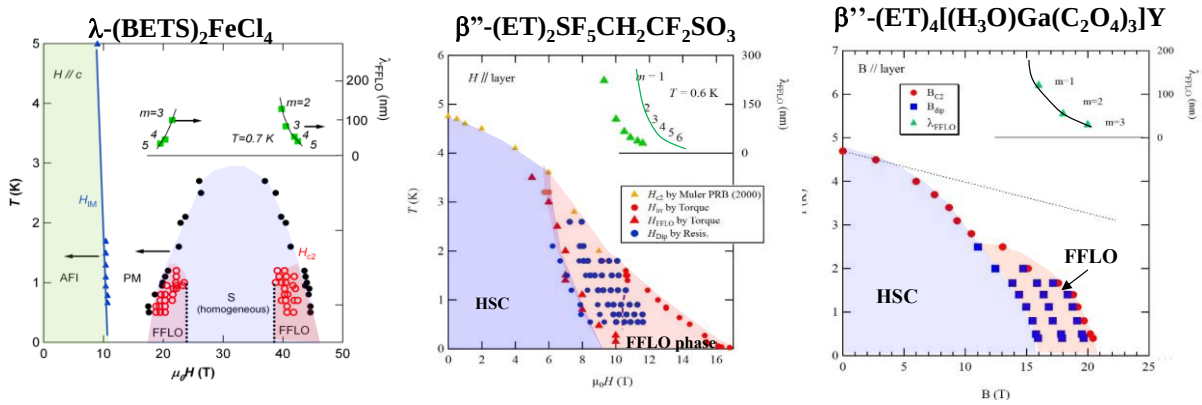


Figure 1: Superconducting phase diagrams for three different organic layered superconductors. Red regions show FFLO phases.

*This work is supported by a Grant-in-Aid for Scientific Research from MEXT, Japan (No. 17H01144).

[1] Uji *et al.*, Phys. Rev. Lett. **97,** 157001 (2006), Phys. Rev. B **85,** 174530 (2012), J. Phys. Soc. Jpn. 82, 034715 (2013), J. Phys. Soc. Jpn. **84**, 104709 (2015), Phys. Rev. B **95**, 165133 (2017), Phys. Rev. B **97**, 144505 (2018).
[2] S. Sugiura *et al.*, npj Quantum Matter **4**, 7, 1 (2019).

Collective mode of the Hidden Order State in URu_2Si_2: Degeneracy and Symmetry

Jonathan Buhot[1], Gregory Setnikar[2], Femke Bangma[1], Mikhail Prosnikov[1], Gérard Lapertot[3], Dai Aoki[3,4], Nigel Hussey[1], and Marie-Aude Méasson[2]

[1]*High Field Magnet Laboratory (HFML-EMFL), Institute for Molecules and Materials, Radboud University Nijmegen, Toernooiveld 7, 6525 ED Nijmegen, The Netherlands*
[2] *Institut Neel, CNRS and Université Grenoble-Alpes, Boite Postale 166, 38042 Grenoble*
[3] *Université Grenoble Alpes, CEA, INAC, PHELIQS, F-38000 Grenoble, France*
[4] *Institute for Materials Research, Tohoku University, Oarai, Ibaraki 311-1313, Japan*

More than thirty years after the discovery of the hidden order (HO) in the heavy fermions compound URu_2Si_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 (Γ_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.

*This work supported by the French Agence Nationale de la Recherche (ANR-DFG "Fermi-NEst" Grant No. ANR-16-CE92-0018, ANR "SEO-HiggS[2]" Grant No. ANR-16-CE30-0014).

1) J. A. Mydosh and P. M. Oppeneer, Reviews of Modern Physics **83**, 1301 (2011).
2) J. Buhot, *et al.,* Phys. Rev. Lett. **113**, 266405 (2014).
3) H.-H. Kung *et al.,* Science **347**, 1339 (2015).
4) J. Buhot *et al.*, Physica B **506,** 19 (2017).

NMR Studies on U-based Ferromagnetic Superconductors

Kenji Ishida[1], M. Manago[1], S. Matsuzaki[1], T. Hattori[1,2], S. Kitagawa[1], Y. Tokunaga[2], K. Deguchi[3], N. K. Sato[3], T. Yamamura[4], Ai Nakamura[5], and Dai Aoki[5]

[1] *Department of Physics, Graduate School of Science, Kyoto University, Kyoto 606-8502*

[2] *ASRC, Japan Atomic Energy Agency, Tokai-mura, Ibaraki 319-1195*

[3] *Department of Physics, Graduate School of Science, Nagoya University, Nagoya 464-8602*

[4]*IMR, Tohoku University, Sendai 980-8577, Japan*

[5]*IMR, Tohoku University, Oarai, Ibaraki, 311-1313, Japan*

Since the discovery of superconductivity in ferromagnet UGe_2 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_{Super} = 0.57 K below FM ordering at T_{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_{Curie} [6]. From the angle-resolved NMR measurements, we found that the magnetic field along the *c* axis ($H \parallel c$) 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 ($H \parallel b$) 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 UTe_2[13], and discuss the similarity and difference in these superconductors.

References

[1] S. S. Saxena *et al.*, Nature **406**, 587 (2000).
[2] D. Aoki *et al*, Nature **413**, 613 (2001).
[3] N. T. Huy *et al*., Phys.Rev. Lett. **99**, 067006 (2007).
[4] T. Ohta *et al.*, J. Phys. Soc. Jpn. **77**, 023707 (2008).
[5] K. Karube *et al.* J. Phys. Soc. Jpn. **80**, 064711 (2011).
[6] Y. Ihara *et al*., Phys. Rev. Lett. **105**, 206403 (2010).
[7] T. Hattori *et al*. Phys. Rev. Lett. **108**, 066403 (2012).
[8] T. Hattori *et al.* J. Phys. Soc. Jpn. **83**, 073708 (2014).
[9] M. Manago *et al*. Phys. Rev. B 99, 020506 (R) (2019)
[10] M. Manago *et al. to be submitted to Phys. Rev. B*
[11] Y. Tokunaga *et al*. Phys. Rev. Lett. **114**, 216401 (2015).
[12] Y. Tokunaga *et al*. Phys. Rev. B **93**, 201112(R) (2016)
[13] Y. Tokunaga *et al. to be submitted to J. Phys. Soc. Jpn.*

Nonsymmorphic topological superconductivity in the paramagnetic superconducting phase of UCoGe

Akito Daido[1], Tsuneya Yoshida[2], and Youichi Yanase[1]
[1]*Department of Physics, Kyoto University, Kyoto 606-8502, Japan*
[2] *Department of Physics, University of Tsukuba, Tsukuba 305-0006, Japan*

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 Z_4 topological phases, which do not appear in the conventional topological periodic table [1]. However, material realization of such 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 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 4π-periodic surface states.

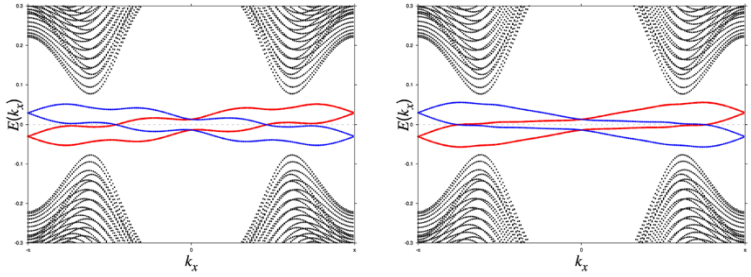


Figure 1:4π-periodic surface states of Z_4 TNCS.

*This work supported by the Local Organizing Committee. Grant-in Aid for Scientific Research on Innovative Areas “J-Physics” (15H05884) and “Topological Materials Science” (16H00991) from JSPS of Japan, and by JSPS KAKENHI Grants No. JP15K05164, No. JP15H05745, and No. JP17J10588, No. JP18H05842, No. 18H01178, and No. 18H05227.

1) X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. **83**, 1057 (2011).
2) K. Shiozaki and M. Sato, Phys. Rev. B **90**, 165114 (2014).
3) K. Shiozaki, M. Sato, and K. Gomi, Phys. Rev. B **93**,195413 (2016).
4) Z. Wang et al., Nature **532**, 189 (2016)
5) P.-Y. Chang, O. Erten, and P. Coleman, Nat. Phys. **13**, 794 (2017)
6) E. Slooten et al., Phys. Rev. Lett. **103**, 097003 (2009).
7) S. Fujimori et al., Phys. Rev. B **91**, 174503 (2015).