ESR studies of the valence bond solid state

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The valence bond solid (VBS) state of the anion radical salt $EtMe_3P[Pd(dmit)_2]_2$ is studied by electron spin resonance (ESR) measurements. The anion layer of $EtMe_3P[Pd(dmit)_2]_2$ is composed of $Pd(dmit)_2$ dimers which is S=1/2, and the dimers form an antiferromagnetic triangular lattice. Although the anion layer is expected to be frustrated, this sample shows a VBS state below 25 K [1]. Hence, we have performed the ESR measurements of $EtMe_3P[Pd(dmit)_2]_2$ to study its spin correlations and spin dynamics.

Firstly, the ESR linewidth shows an unconventional angular dependence, at 4 K which can only be explained by the lack of interlayer interaction between the $Pd(dmit)_2$ dimers (Fig. 1). However, this lack of interlayer interaction contradicts with recent *ab-initio* calculations. Meanwhile, the integrated intensity of ESR signals, which is proportional to the spin susceptibility, decreases gradually by lowering the temperature and becomes constant at 25 K (Fig. 2). This behavior suggests that spin singlet is gradually created by lowering the temperature, but some spins remain below 25 K. We suppose the lack of the interlayer interaction is due to the long distance between the residual spins. Detailed analysis of the ESR measurements will be presented and discussed.

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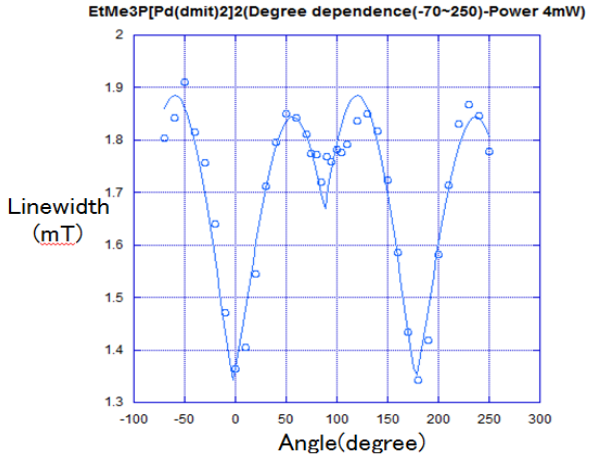

Fig. 1. Angular dependence of linewidth at 4 K for B//*ab*-plane.

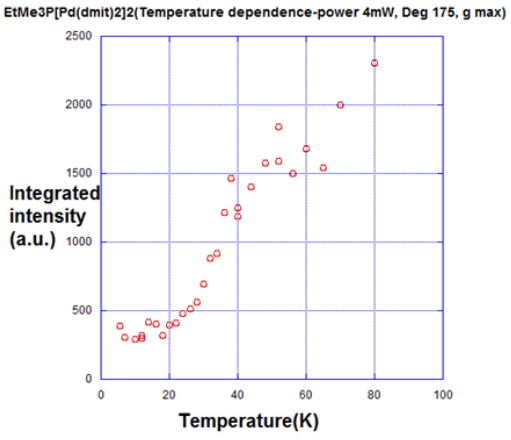

Fig. 2. Temperature dependence of the ESR integrated intensity for B//b^*-axis.

Investigation of magnetic ordered states in the $(Nd_{1-x}Ca_x)_2Ir_2O_7$ probed by μSR

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The correlated electron (U) and nontrivial physics from spin-orbit coupling (SOC) are two two central threads of quantum materials to realize many exotic phases, such as Axion insulator, Weyl semimetal, and topological Mott insulator [1]. Typical systems which have comparable U and SOC are pyrochlore iridates. Interestingly, in these pyrochlore systems, U can be systematically tuned by changing ionic radius of R^{3+} ion (r) [1]. As r increases, the temperature of metal-insulator transition (MIT) gradually decrease, and its boundary lies between R = Nd and Pr [2]. An abundant of emergent quantum states has been theoretically predicted on the boundary of MIT [1]. Accordingly, to unravel those states, it is necessary to control U more finely in the MIT critical region, which can be achieved by chemical substitution on $Nd_2Ir_2O_7$.

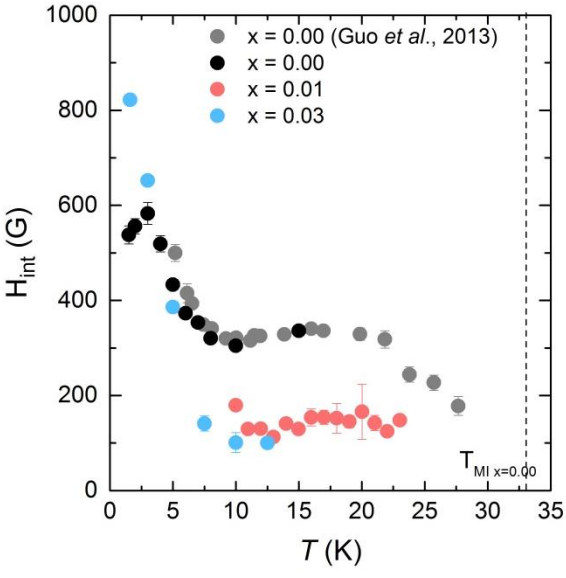

Fig.1. The internal field dependence of temperatures in $(Nd_{1-x}Ca_x)_2Ir_2O_7$

In this study, we report the effect of Ca substitution on the magnetically ordered state of Ir^{4+} moments in $Nd_2Ir_2O_7$ investigated by muon-spin relaxation. $Nd_2Ir_2O_7$ shows metallic behavior at high temperature, and undergoes MIT at temperature of T_{MI} = 33 K [2]. In our previous μSR study, we observed the appearance of long-range magnetically ordered state of Ir^{4+} moments at temperature cooperated with T_{MI} [3]. The addition of hole carrier via Ca substitution gradually decreases the magnetic transition (T_M), as well as T_{MI}, and suppresses the onset of magnetically ordered state. As shown in the Figure 1, Ca substitution suppresses the magnetic ordered states Ir^{4+} moments, while the additional long-range order of Nd^{3+} moments appears below 10 K. Detail results of the μSR measurements on $(Nd_{1-x}Ca_x)_2Ir_2O_7$ will be presented in the talk.

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Persistent chimera states in nonlocally coupled phase oscillators

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In the systems of nonlocally coupled identical limit-cycle oscillators, there often appears an interesting phenomenon called the chimera state. The chimera state is characterized by the coexistence of coherent and incoherent regions as shown in Fig. 1. The coherent region of the chimera state consists of synchronized oscillators with the identical average frequency, while the incoherent region consists of not-synchronized oscillators.

We consider the system of nonlocally coupled phase oscillators

$$\dot{\theta}_j(t) = \omega + \frac{1}{2R}\sum_{k=j-R}^{j+R} \Gamma(\theta_j(t) - \theta_k(t)), \tag{1}$$

where θ_j $(j = 1, \ldots, N)$ is the phase of ith oscillator, ω is the identical natural frequency and R is the coupling range. As the 2π-periodic coupling function Γ, the sine coupling $\Gamma(\phi) = -\sin(\phi + \alpha)$ is generally used, where α is the phase lag parameter. In the continuous limit $N \to \infty$, the chimera state is a stable steady state [1]. However, in the finite N cases, the chimera state for the system (1) with the sine coupling is chaotic transient and finally collapse into the completely synchronous state [2].

In this study, we have investigated the chimera state in the system (1) with the Hansel-Mato-Meunier coupling $\Gamma(\phi) = -\sin(\phi + \alpha) + r\sin(2\phi)$, where r is the amplitude ratio of the second harmonic component, and obtained the result that the chimera state in the finite N case can be persistent (nontransient) by the numerical simulation. Details of this study was already published as [3].

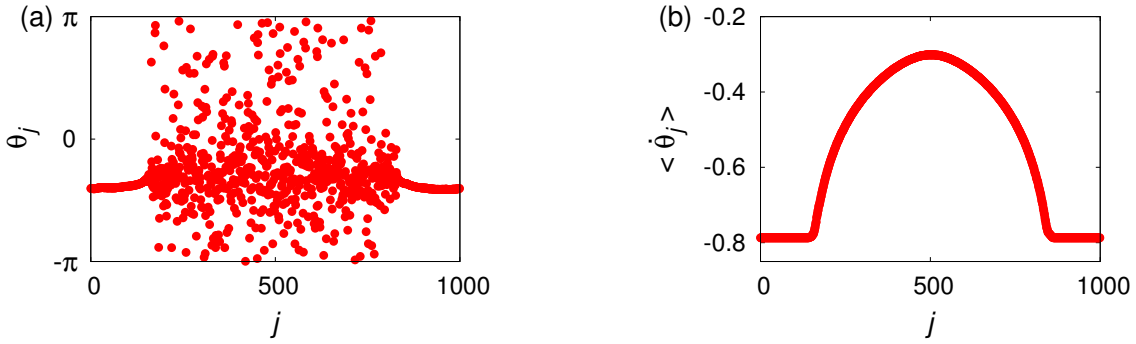

Figure 1: The chimera state for the system (1) with $N = 1000$. The left figure shows the snapshot of phase θ_j, and the right figure shows the profile of the average frequency $\langle\theta_j\rangle$.

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[3] Y. Suda and K. Okuda, Phys. Rev. E **92**, 060901(R) (2015).

Induced Charge-Density-Wave in Cu-doped $TaSe_3$

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Induction of states is helpful in understanding their mechanism and searching their new characters as we can see in high-temperature superconductors and the sulfur hydride system. If a Charge-Density-Wave (CDW) is induced in materials which do not exhibit a CDW, new CDW properties might be brought there. Transition metal trichalcogenides (MX_3) are quasi-one-dimensional conductors due to their chain structure. In most of MX_3 ($NbSe_3$, TaS_3, NbS_3), CDWs occur under the transition temperature. On the other hand, $TaSe_3$ exhibits no CDW transition. The cause has been considered that $TaSe_3$ is more three-dimensional than the other MX_3 compounds. Conversely considering, if we can expand the distance between chains and make the dimension lower by doping, a CDW may be induced also in $TaSe_3$.
Therefore, we tried to induce a CDW in $TaSe_3$ by doping Cu. By measuring the resistance as a function of temperature, the dip of the temperature derivative of resistance was observed in Cu-doped $TaSe_3$, not in pure $TaSe_3$. The dip of the temperature derivative of resistance indicates a phase transition with the rise of resistance, suggesting that a CDW is induced in $TaSe_3$ by Cu-doping. The single-crystal X-ray diffraction pattern (XRD) implies that the *a*- and *c*-axis lattice parameter are expanded and *b*-axis lattice parameter is contracted by Cu-doping. The increase of electrical conductivity anisotropy linking with the change of lattice parameters might make nesting of the Fermi surface good and as a result, a CDW might be induced.

Magnetic Ground State of CeT_2Al_{10} (T = Ru, Os)

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The Ce-based compound, CeT_2Al_{10} (T = Ru, Os) is a Kondo semiconductor that exhibits an unusual high transition temperature at T_N ~ 30 K which is still under debatable [1]. The system shows strong magnetic anisotropy ($\chi a > \chi c > \chi b$) with a small ordered moment, 0.42 μ_B which contrarily aligns along the *c*-axis [2]. In the case of electron doping by the substitution of Rh for Ru, spin-flop from *c*-axis to *a*-axis occurred with a larger amount of magnetic moment, 1.06 μ_B after 5% of Rh doping [3]. An investigation by muon spin spectroscopy (μSR) shows a drastic change of internal field from 170G in $CeRu_2Al_{10}$ to 780 G after 3% of Rh doping [4]. However, different spin-flop behaviour from *c*-axis to *b*-axis was observed in the case in substitution of 5% La for Ce, $(Ce_{1-x}La_x)Ru_2Al_{10}$. The transition temperature also decreased consistently accompanied by a decrease of magnetic moment as the La concentration increased more than 7%. Conversely, the same spin-flop behaviour couldn't be observed in $(Ce_{1-x}La_x)Os_2Al_{10}$ system [5].

We investigated magnetic ground state of $(Ce_{1-x}La_x)T_2Al_{10}$ (T = Ru, Os) using μSR. Both compounds exhibited clear sign of coherent oscillation in the time spectrum at low temperature confirming the appearance of a long-range magnetically ordered state Ce moments. However, no critical changes found in the internal field suggesting no spin-flop behaviour occur. In addition to those experimental efforts, we carried out computational analysis of muon sites in $CeRu_2Al_{10}$ and examined the electronic state of Ce moments around muon in order to study the spin-flop behaviour.

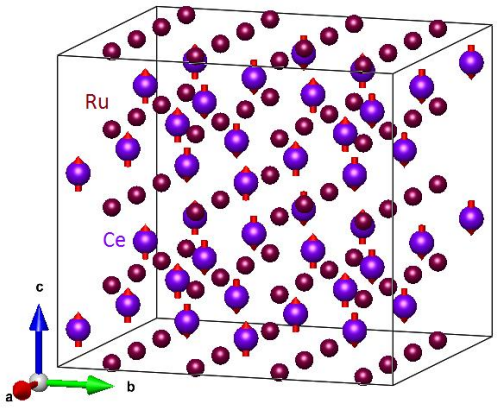

Figure 1: Spin structure of Ce-ion in the magnetically ordered state estimated from our computational investigations by using the density functional theory.

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Intrinsic spatial dependence of superconducting gap in high-T_c cuprate $Bi_2Sr_2CaCu_2O_{8+\delta}$: an STM/STS study

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One of the interesting features of Bi-based high-T_c cuprates such as $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212) is the one-dimensional (1D) superlattice structure along the *b*-axis (forming a slant angle of 45° from the Cu-$O_{inplane}$ bond direction), modulating the bond length between the Cu and the apical O (O_{apical}) atoms of CuO_5 pyramids [1], which has been considered to cause a periodic modulation of the antiferromagnetic (AFM) coupling between Cu-spins $J(\boldsymbol{r})$ [2]. The 1D superlattice period ~ 26 Å is similar to the superconducting (SC) coherence length of this system; therefore, it may affect local properties of superconductivity [2]. In this study, to clarify the effect of such a superlattice structure on the high-T_c superconductivity, we performed STM/STS experiments on cleaved surfaces of nearly optimal Bi2212 crystals with T_c=90 K and examined the spatial dependence of the SC gap (SCG).

In many cases of STM/STS experiments on Bi2212 cleaved surfaces, STS spectra exhibit a two-gap structure consisting of a *d*-wave SCG and a spatially inhomogeneous pseudogap (PG), the so-called "large PG," whose size varies in nanometer scale over a wide range from an energy of the *d*-wave SCG amplitude Δ_0 to several times larger one [3, 4]. Furthermore, a checkerboard-type charge order (CCO) is observed on Bi2212 cleaved surfaces that are accompanied by the inhomogeneous large PG [4]. On some cleaved surfaces used in the present study, however, an STS spectrum consistent with a single *d*-wave like SCG structure, together with no CCO, was observed at every measurement point within the areas examined at 8 K. It is characterized by sharp peaks at bias voltages V_s corresponding to the gap edges $V_s = \pm\Delta_0/e$. This enabled us to examine and demonstrate the intrinsic spatial dependence of SCG in Bi2212: (1) the *d*-wave like SCG modulates along the *b*-axis with the same period as the 1D superlattice or $J(\boldsymbol{r})$, and (2) the amplitude of the modulation is ~5% of its average value, which probably suggests a correlation between the SCG and the AFM coupling of Cu-spins. We will also report a correlation between SCG size and a characteristic energy of an AFM resonance mode of Bi2212.

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Vortex-core charging due to the Lorentz force in a *d*-wave superconductor

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We still have quite a poor understanding of the Lorentz force on the supercurrent and related phenomena. This is because the force on supercurrent itself may easily be overlooked in the presence of the predominant diamagnetic effect by supercurrent obeying Ampere's law. Indeed, the Lorentz force is missing from the standard Ginzburg-Landau and quasiclassical Eilenberger equations that have been used extensively to study superconductors theoretically. Hence, physics of the Lorentz force in superconductors remains mostly unexplored theoretically.

We derive augmented quasiclassical equations of superconductivity with the Lorentz force in the Matsubara formalism so that the charge redistribution due to supercurrent can be calculated quantitatively[1]. Using it, we obtain an analytic expression for the vortex-core charge of an isolated vortex in extreme type-II materials given in terms of the London penetration depth and equilibrium Hall coefficient. It depends strongly on the Fermi surface curvature and gap anisotropy, and may charge sign even as a function of temperature due to the variation in the excitation curvature under the growing energy gap. This is also confirmed in our numerical study of high-T_c superconductors.

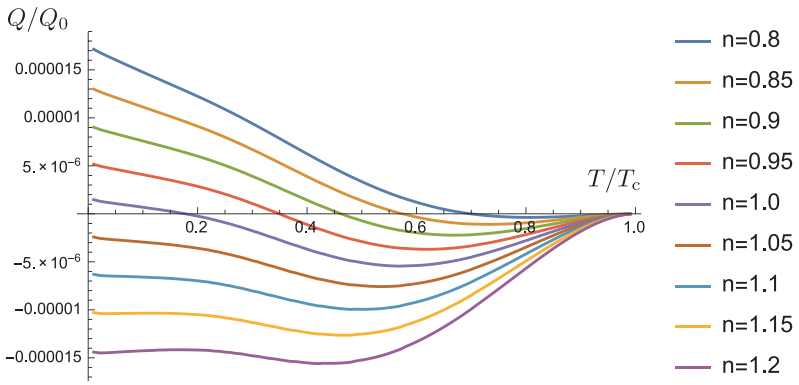

Fig.1 Temperature dependence of the vortex-core charge. n is the electron filling.

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μSR Study Of Organic Superconductor λ-$(BETS)_2GaCl_4$

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Dita Puspita Sari

The conducting organic system λ-$(BETS)_2$ $Fe_xGa_{1-x}Cl_4$ is a hybrid system which consists of π electrons of BETS molecule and 3*d* ones on Fe ions. In the zero-field condition, λ-$(BETS)_2FeCl_4$ shows the metal-insulator transition at ~8 K and becomes superconducting with the transition temperature, $T_c \cong 5$ K in 33 T, while λ-$(BETS)_2GaCl_4$ is superconducting with $T_c \cong$ 5-6 K even in zero field [1]. In order to achive deeper understanding on those superconducting states, studies on isostructural λ-$(BETS)_2GaCl_4$ are important but less studies have been done on this system [2-3]. Specific heat measurement macroscopically suggested a *d*-wave pairing symmetry [4]. Accordingly, we carried out muon-spin relaxation (μSR) mesurement on λ-$(BETS)_2GaCl_4$ down to 0.3 K at the RIKEN-RAL Muon Facility.

From zero-field (ZF) μSR, it was found that the muon-spin relaxation rate was independent of temperature even in the superconducting state. This means that the time-reversal symmetry of the superconducting state would not be broken. Figure 1 shows the temperature dependence of the muon-spin depolarization rate measured in the transverse-field (TF) of 30 G. The TF was applied in perpendicular to the muon spin direction. The depolarization rate starts to increase just below T_C and have a round shape around 2 K. The tendency suggest that it was not simple *d*-wave nor *s*-wave.

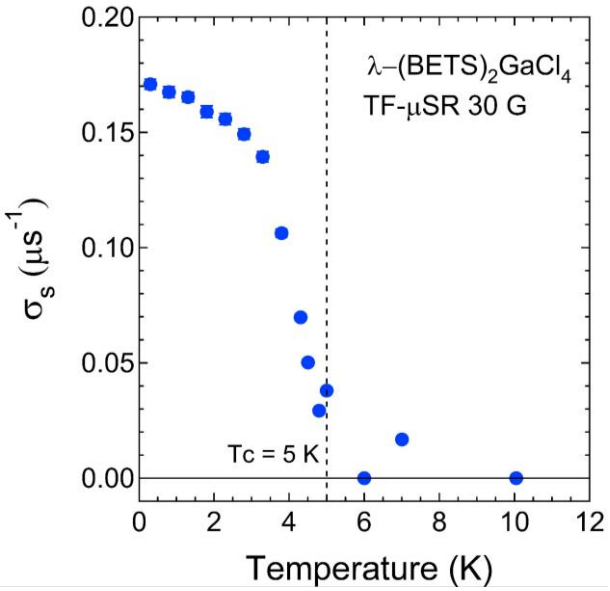

Figure 1. Temperature dependence of the muon-spin depolarization rate measured on λ-$(BETS)_2GaCl_4$ in the transverse field of 30 G.

References:

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μSR and DFT+U Studies of High-Tc Superconductor Cuprates

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It is different from conventional superconductors which don't like magnetics fields, cuprates superconductor perform the coexistence of magnetism and superconductivity [1], and furthermore magnetism in cuprates superconductor may play role in driving pairing mechanism [2]. *Muon-Spin Rotation and Relaxation* (μSR) is one of most sensitive instruments to study the magnetism of cuprates supercondutor such as spin-spin correlation, spin density wave, spin fluctuations and spin-flop transition However, to get more quantitatively interpretation of μSR data, it is needed to know the precisely stopping site on muon in the material. The estimation of muon site in some cuprates superconductor material by both Hatree-Fock and Density Functional Theory (DFT) calculations has been done in some previous works [3-6], nevertheless the studies have not treated yet the materials as strongly correlated system which exhibits Mott-insulator behaviour.

In our proposed research, we will reinvestigate the muon stopping site in cuprates superconductor material by using the Hubbard-rooted Density Functional Theory (DFT+U) method by Anisimov *et al* [7,8]. The location muon in cuprates material is assumed at minimum electrostatic potentials, and it will be studied for both with or without the change of internal structure cases taking into account the zero-point energy of muon vibration. We will also study cuprates material with or without doping to see the dependence of magnetic order on dopant concentration.

Our expectated results are that besides providing antiferromagnetic insulator behaviour shown by the existence of gap energy and zero total magnetic moments as well as the magnetic phases of doped cuprates material, the Hubbard correction will also effect the the distribution of spin density, so it will refine the previous calculation on internal fields.

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^{13}C NMR study of nonmagnetic insulating phase of λ-(BEDT-STF)$_2$GaCl$_4$

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Quasi-two-dimensional organic conductors λ-(BETS)$_2$*M*Cl$_4$ (*M*=Ga, Fe) [BETS: $C_{10}H_8S_4Se_4$] which have attracted attention because, these salts show novel features of superconductivity including Fulde-Ferrell-LarkinOvchinnikov (FFLO) and magnetic field-induced superconductivity (FISC) [1-4]. In λ-(BETS)$_2$GaCl$_4$, *d*-wave SC gap structure was reported by a specific heat measurement[5], however, superconducting (SC) paring mechanism of λ salts is still unclear due to lack of universal phase. To clarify what fluctuation the superconductivity mediates in strongly correlated electron system, electron correlation in insulating phase near the SC phase is important. Recently, it is revealed that insulating phase of λ-(BEDT-STF)$_2$GaCl$_4$ [BEDT-STF: $C_{10}H_8S_6Se_2$] is located in vicinity of λ-(BETS)$_2$GaCl$_4$. Therefore, λ-(BEDT-STF)$_2$GaCl$_4$ is appropriate material for studying electron correlation in insulating phase.

We investigated magnetic property of insulating phase of λ-(BEDT-STF)$_2$GaCl$_4$ by site-selective ^{13}C NMR. Large enhancement of $(T_1T)^{-1}$ was observed below 20 K as shown in Fig. 1, indicating strong AF spin fluctuation exits. We also observed anomalous decrease of linewidth, although long-range magnetic ordering did not occur. We will report the results in more detail in this presentation.

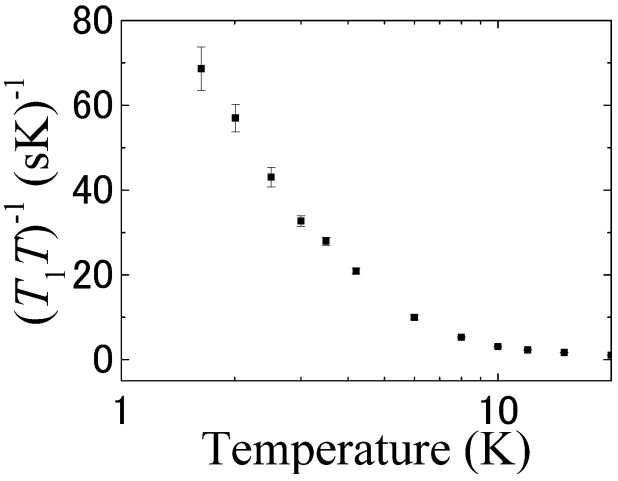

Fig.1 Temperature dependence of $(T_1T)^{-1}$.

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Magnetic property of a honeycomb ruthenate α-$RuCl_3$ investigated by spin polarized muons

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The honeycomb ruthenate, α-$RuCl_3$, was suggested as a candidate to realize Kitaev spin model with those reasons, such as the cubic environment surrounded by Cl-ions for the strong spin orbit coupling, and honeycomb layers connected by a weak van der Waals interaction for the ideal two dimensional environment to cause the bond dependent exchange[1].

We synthesized honeycomb ruthenate single crystal. This material shows the rhombohedral lattice in the the crystal structure survey, and exhibits the single magnetic anomaly, 6 K, 9.5 K, and 12.5 K in the DC susceptibility results as shown in Fig. 1. This result is similar with the previous experimental results[2-4].

In order to get the information of details of magnetic behaviors, we carried out μSR measurements at the RIKEN-RAL Muon Facility with the α-$RuCl_3$ single crystal. We are going to present the magnetic ordered behavior around 6 K at zero field. Also, we will talk about the spin dynamics of the α-$RuCl_3$ around 6 K revealed in the longitudinal field dependence.

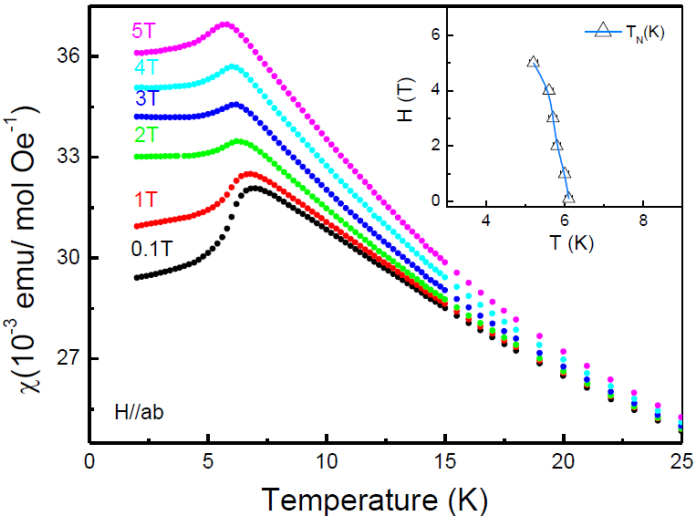

Fig.1 Temperature dependence of DC susceptibilities at various fields.

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Magnetic Properties in Organic π-d System

λ-(BEDT-STF)$_2$FeCl$_4$

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Quasi-two-dimensional organic conductor λ-(BETS)$_2$FeCl$_4$ (BETS = bis(ethylenedithio)tetraselenafulvalene) is well-known as the first organic material to show magnetic-field induced superconductivity [1]. This salt shows metal-AF insulator transition at 8.3 K at zero magnetic field [2]. Magnetization measurements have shown that the Fe^{+3} ion is found in the S = 5/2 high-spin state, and it has been believed so far that the metal-AF transition is due to the AF ordering of the Fe moments. However, based on thermodynamic properties a recent study proposed that the 3*d*-spin state is paramagnetic and the pi-spin state is AF ordered [3]. The questions regarding the mechanism of AF transition are still unanswered.

To elucidate the mechanisms of AF insulating phase, we conducted ^{1}H-NMR and magnetic susceptibility measurements for λ-(BEDT-STF)$_2$FeCl$_4$ (BEDT-STF = bis(ethylenedithio)diselenadithiafulvalene), which can be placed at the negative pressure region of BETS salt. We observed the sharp peak in the $1/T_1$ and broadening of the NMR spectrum, which associate to the AF transition, at 16 K. We also found that the magnetic susceptibility showed a broad peak structure at 8 K and there was no anomaly at 16 K. Furthermore, in the K-χ plot, the NMR shift shows the enormous increasing in AF phase.

We concluded that the spin susceptibility in AF state in these salts can be explained in the framework with AF ordered π-spin system, however, we must take into account the finite *d*-*d* AF interaction toward a detailed understanding of the behavior of 3*d*-spin system.

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Superconducting pairing gap due to orbital nematic fluctuations

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In iron-based superconductors, superconductivity (SC) is realized close to the magnetic phase [1]. In addition, the so-called electronic nematic phase, which breaks only the orientational symmetry and retains the other symmetries, is usually realized also close to the magnetic phase. As a result, SC occurs closer to the nematic than the magnetic phase. Hence nematic fluctuations are expected to play an important role for SC. As the origin of nematic fluctuations, spin and orbital nematic scenarios are discussed. In this study, we focus on the latter scenario and study SC from orbital nematic fluctuations.

We already have theoretical works on SC from orbital nematic fluctuations. Yanagi *et al.* studied Eliashberg equations and found that the symmetry of the superconducting gap becomes s_{++}-wave [2]. However, the renormalization of quasiparticles was not considered. Consequently, obtained T_c became unrealistically high and SC was realized slightly above the onset temperature of the nematic phase, in contrast to experimental observations. Yamase and Zeyher overcame these drawbacks by including the renormalization function [3]. They found that orbital nematic fluctuations drive strong coupling SC and T_c becomes comparable to experimental values, implying that orbital nematic fluctuations can be a new mechanism of high-T_c SC. The superconducting gap is, however, assumed constant on each Fermi surface.

In this study, we develop the analysis of Eliashberg equations by allowing a momentum dependence of the gap and aim to establish a new high-T_c mechanism from orbital nematic fluctuations. When SC occurs from the tetragonal phase, we find that the superconducting gap exhibits a weak momentum dependence and can be approximated to be isotropic s_{++}-wave. SC can occur also inside the nematic phase. In this case, the superconducting gap retains s_{++}-wave symmetry, but can become highly anisotropic. The momentum dependence of the gap is understood by considering orbital components on each Fermi surface. We discuss a possible relevance to a recent angle-resolved photoemission spectroscopy data [4].

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Theory of magnetic Raman scattering in antiferromagnetic spin tubes

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Magnetic Raman scattering - inelastic photon scattering by magnons - is important probe to study magnetic excitation of antiferromagnets and there are many experimental observations and theoretical calculations[1]. Magnetic Raman operator is described as "photo-induced" exchange interaction[2, 3] like equation(1).

$$\mathcal{R} = \sum_{\boldsymbol{r}} \sum_{\boldsymbol{\delta}} \Lambda_{\boldsymbol{\delta}} (\hat{\boldsymbol{e}}_{\mathrm{i}} \cdot \boldsymbol{\delta})(\hat{\boldsymbol{e}}_{\mathrm{s}} \cdot \boldsymbol{\delta}) \boldsymbol{S}_{\boldsymbol{r}} \cdot \boldsymbol{S}_{\boldsymbol{r}+\boldsymbol{\delta}} \tag{1}$$

Here, $\Lambda_{\boldsymbol{\delta}}$ is proportional to exchange interaction, $\hat{\boldsymbol{e}}_{\mathrm{i}}(\hat{\boldsymbol{e}}_{\mathrm{s}})$ is polarization vector of incident(scatterd) light, $\boldsymbol{\delta}$ is the vector which connect the two site, and $\boldsymbol{S}_{\boldsymbol{r}}$ is spin operator of site $\boldsymbol{r}$. We evaluate dynamical correlation function of equation(1).

We investigated magnetic Raman scattering properties of $\mathrm{D_{4h}}$ symmetry square prism antiferromagnetic Heisenberg spin tube (FIG.1) by modified spin wave theory[4]. With increase of $J_{\parallel}/J_{\square}$, where $J_{\parallel}$ and $J_{\square}$ are exchange interaction on the tube leg and square plaquette respectively (see FIG.1), peak positions shift to higher energy side and structure of spectrum changes single peak to double peak (FIG.2). Changes of the spectrum reflect change of dispersion relation, so we can estimate the magnetic structure of spin tube from $\mathrm{B_{1g}}$ mode magnetic Raman spectrum. In the presentation, we will report more detail which include dependence of polarization direction of light.

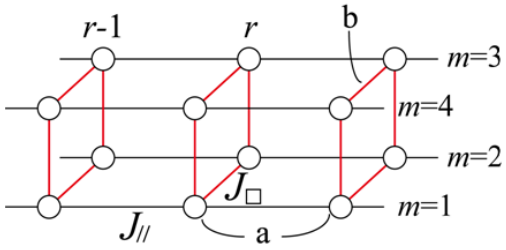

FIG.1 Schematic picture of $\mathrm{D_{4h}}$ square prism spin tube.

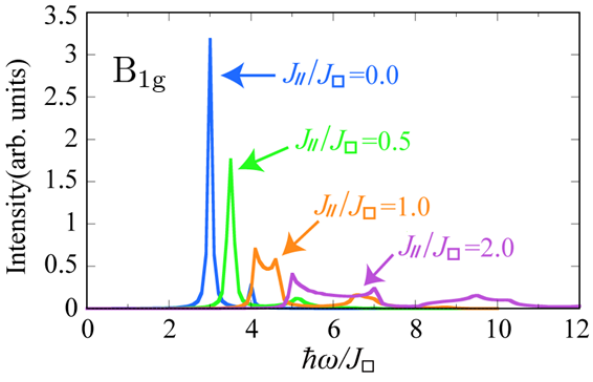

FIG.2 Dependence of ratio of exchange interaction $J_{\parallel}/J_{\square}$ in $\mathrm{B_{1g}}$ mode magnetic Raman spectrum at $T = 0K$.

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Magnetic properties of the molecular bi-layer materials

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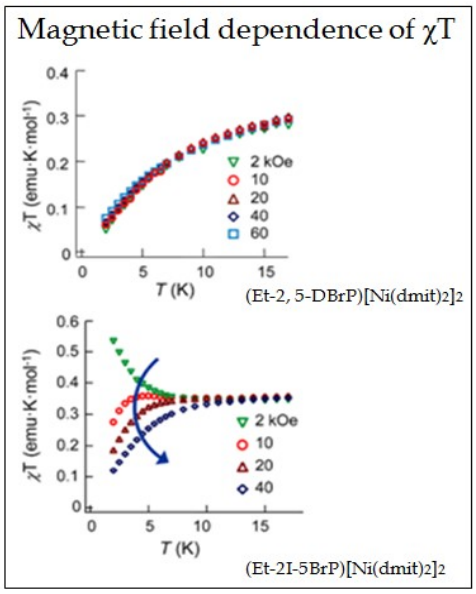
Recently, a novel bi-layer Mott materials, (Et-2,5-DBrP)$[Ni(dmit)_2]_2$ (Et=ethyl, DBrP=dibromopyridinium) and (Et-2I-5BrP)$[Ni(dmit)_2]_2$ (BrP=bro mopyridinium), have been synthesized [1]. These salts have two crystallo-graphically independent anion layers in the unit cell thanks to the asymmetric shape of the cations and the halogen bonding between the cation and the anion. The $Ni(dmit)_2$ molecules are strongly dimerized for each layer, and the system is expected to be a Mott insulator. Actually, these two salts are insulating down to the lowest temperature. However, its magnetic properties show uncon-ventional features not seen in regular Mott system.

Firstly, both salts do not show any sign of magnetic long-range order. Secondly, although the temperature dependence of χT for (Et-2,5-DBrP) $[Ni(dmit)_2]_2$ shows an antiferromagnetic property, where χT decreases with decreasing temperature, the temperature dependence of χT for (Et-2I-5BrP)$[Ni(dmit)_2]_2$ shows more complex magnetic properties, where the temperature dependence of χT shows a ferromagnetic behavior at low field but changes to an antiferromagnetic behavior above 1 T. It is worth to stress that such difference of the magnetic properties is just created by the small change of cations. Namely, one bromine of (Et-2,5-DBrP) is just substituted by iodine.



Magnetic properties of (Et-2,5-DBrP)$[Ni(dmit)_2]_2$ (top) and (Et-2I-5BrP)$[Ni(dmit)_2]_2$ (bottom) by T. Kusamoto *et al.* Ref. [1]

It is supposed that the signs of intralayer and interlayer exchange interactions play an important role in the magnetic properties of the bi-layer salts [1]. From the temperature dependence of χT, it is expected that intralayer exchange couplings are antiferromagnetic for both salts, but interlayer exchanges are antiferromagnetic and ferromagnetic for (Et-2,5-DBrP)$[Ni(dmit)_2]_2$ and (Et-2I-5BrP)$[Ni(dmit)_2]_2$, respectively. However, this is just a speculation from the macroscopic magnetic measurements, and microscopic measurements that directly probe the spins are highly anticipated. Therefore, we will investigate the bi-layer materials using ESR spectroscopy.

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Muon sites calculation on $YBa_2Cu_3O_6$

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Since the discovery of high-T_c superconductivity, a large number of investigation, both experimental and theoretical have been carried out in this exciting field to understand the different aspect of these system. One of the high-T_c superconductivity is $YBa_2Cu_3O_{6+x}$ (YBCO) compound and also well known as 123 compound. The electromagnetic properties of YBCO can be controlled by controlling the oxygen content *x*. When $x = 0$, an insulating YBCO in magnetically ordered state and as we increase the *x*, magnetic order state disappears and superconducting state appear at $x > 0.4$ and it has a transition temperature T_c of about 90 K.

Previously, neutron diffraction experimental had suggested Cu2 has magnetic moment $0.66\mu_B$ antiferromagnetically[1] and the zero field muon spin rotation and relaxation (ZF-μSR) on $YBa_2Cu_3O_{6.2}$ indicates the existence of long range magnetic order below room temperature has internal field 300 G.[2] μSR internal field had suggested that muon will stop at two sites, near apical oxygen and planar oxygen.[2]

In order to clarify the muon site, we have performed an *ab-initio* density functional theory (DFT) calculation for muon implanted in YBCO. We estimated muon site from the view point of potential energy[3] by using VASP program taking into account the relaxation atoms and the muon sites. Based on the potential calculation, we have calculated the dipole field at the muon site including the relaxation atoms, then the dipole field calculation results will be compared with the internal field at muon sites by experimental.

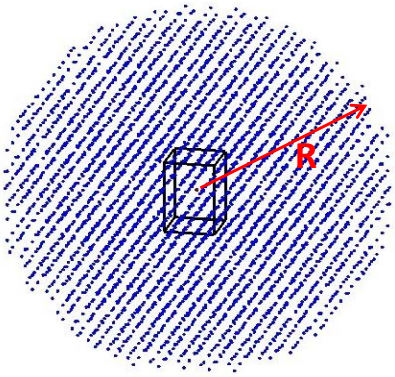

Fig.1 The dipole field model. R is the distance between muon and the outer atoms.

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Magnetic Order of π-electrons in the Alkali Metal Superoxide of CsO_2 studied by the Muon Spin Resonance

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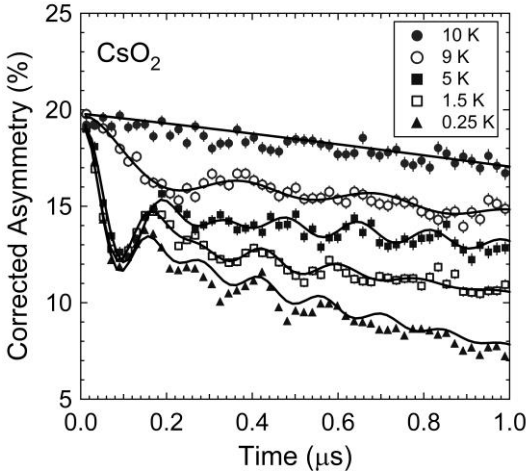
Alkali metal superoxides (AO_2) such as NaO_2, KO_2, RbO_2, and CsO_2 are ideal model systems for the study of *p*-electron magnetism. The KO_2 and RbO_2 systems have already been well studied and exhibit antiferromagnetic behavior at the temperature of 7 K and 15K respectively. However, CsO_2 has been less investigated due to the difficulty in synthesizing samples. All AO_2 compounds undergo structural distortions splitting the degeneracy of the π^* orbitals and creating an orbitally ordered state. From an NMR study on CsO_2, Tomonaga-Luttinger liquid behavior was suggested to appear below about 70 K where an antiferromagnetic spin chains is formed as a result of the *p*-orbital ordering. A magnetically ordered state is expected to appear below about 10 K in CsO_2 [1,2].

Based on the μSR result, in the ZF condition, the long range magnetic order appear below 10 K. The frequency of muon spin precession is higher with the decreasing of temperature indicating the growth of internal field on muon sites. For further analysis, WIMDA program is used to get the fitting function and some parameter. In order to get more detail information, the DFT calculation is carried out to estimate the muon stopping position. There are 2 possible muon positions around O_2^- dumbell.



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