APCTP-Quantum Materials Symposium 2017

in conjunction with 17th Korea-Taiwan-Japan Workshop on SCES & APW

Program & Abstracts

February 19 (Sun), 2017 ~ February 24 (Fri), 2017

Yongpyong Resort (Dragon Valley Hotel), Korea

미래창조과학부 Ministry of Science, ICT and Future Planning
복권위원회
NRF 한국연구재단
APCTP Asia Pacific Center for Theoretical Physics
CTP Center for Theoretical Physics
CQMS
IBS CCES Center for Correlated Electron Systems
IBS 기초과학연구원

Overview

APCTP-Quantum Materials Symposium 2017 (QMS17) is organized by the Korean condensed matter physics community of strongly correlated electron systems (SCES) and various institutes in Korea including Asia-Pacific Center for Theoretical Physics (APCTP), IBS (Institute of Basic Science) Center for Correlated Electron Systems (IBS-CCES) and IBS Center for Artificial Low Dimensional Electronic Systems (IBS-CALDES). QMS17 will be held together with APW and 17th Korea-Taiwan-Japan Workshop. We intend to bring world-renowned researchers in various frontiers in condensed matter physics.
In keeping with our tradition of hosting the symposium in a relaxed atmosphere, we hold APCTP-QMS17 at Yongpyong Ski Resort during Feb. 19-24, 2017.

Scope

During the six-day symposium, we hope to cover various topics in condensed matter physics such as quantum magnetism, unconventional superconductivity, heavy fermion, quantum phase transition, low-D electronic materials, etc…

Organizers

Chair – Tuson Park (Sungkyunkwan Univ.)
Vice Chair – Kee-Hoon Kim (Seoul National Univ.)
Organizing committee:
Yunkyu Bang (Chonnam National Univ.)
Gun-Sang Jeon (Ewha Womans Univ.)
Younjung Jo (Kyungpook National Univ.)
Jung Hoon Han (Sungkyunkwan Univ.)
Changyoung Kim (Seoul National Univ.)
Jun Sung Kim (IBS-CALDES, POSTECH)
Tae-Hwan Kim (POSTECH)
Jae-Hoon Park (POSTECH)
Je-Geun Park (Seoul National Univ.)
Kwon Park (KIAS)
Chan-Ho Yang (KAIST)
Jaejun Yu (Seoul National Univ.)

Timetable

	Feb 19 (Sunday)	**Feb 20** (Monday)	**Feb 21** (Tuesday)	**Feb 22** (Wednesday)	**Feb 23** (Thursday)	**Feb 24** (Friday)
Morning Ⅰ (09:00-10:30)	**SUN 1** Andeas Heinrich Shik Shin Di-Jing Huang	**MON 1** Hidenori Takagi Jae Hoon Kim Kenya Ohgushi	**TUE 1** Jan Zaanen Sang-Jin Sin	**WED 1** J. D Thompson S Wirth P Riseborough	**THU 1** F Ronning K Ishida Ji Hoon Shim	**FRI 1** S.-W. Cheong J Knolle SungBin Lee
	Break					
Morning Ⅱ (11:00-12:30)	**SUN 2** Ying-Hao Chu Tae Heon Kim Ming-Wen Chu	**MON 2** Takuro Katsufuji Suyeon Cho Guang-Yu Guo	**TUE 2** Choong H. Kim Mehdi Biderang Wen Hong Wang	**WED 2** P Gegenwart J Denlinger K Kanoda	**THU 2** Y Kim T Hanaguri Seung-Ho Baek	**FRI 2** K Choi M Hermanns
	Lunch					Closing
Afternoon Ⅰ (14:00-15:30)	**SUN 3** Jan-Chi Yang Tsuyoshi Kimura Cheng-Maw Cheng	**MON 3** Atsushi Fujimori Jae Hoon Park Ashish Atma	**TUE 3** Xi Dai Shuich Murakami Susk Bum Chung	**WED 3** M Grosche Sun-Sik Lee S Hasegawa	**THU 3** Jun Sung Kim J. G. Analytis Tae-Hwan Kim	
	Break					
Afternoon Ⅱ (16:00-17:30)	**SUN 4** Poster Session Ⅰ	**MON 4** Y.Motome Jaejun Yu	**TUE 4** Shun-Qing Shen S.A. Jafari Fu-Chun Zhang	**WED 4** Poster Session Ⅱ	**THU 4** H.-S. Sim K Burch	
18:00		**Banquet** (all Participants)			**Dinner** with Invited Speakers	

Session SUN 1

Chair: Prof. Je-Geun Park

09:10-09:40 Andreas Heinrich (Ewha Womans Univ.), "Electron Spin Resonance of single atoms on a surface"

09:40-10:10 Shik Shin (Tokyo Univ.), "Laser-PEEM study on the photo-induced ferromagnetism in $SrTiO_3$ surface"

10:10-10:40 Di-Jing Huang (NSRRC), "Spin crossover of cobaltates revealed by resonant inelastic X-ray scattering"

Session SUN 2

Chair: Prof. Atsushi Fujimori

11:00-11:30 Ying-Hao Chu (National Chiao Tung University), "Flexible Oxide Heteroepitaxy: A New Playground for Exploring Intriguing Properties of Functional Oxides"

11:30-12:00 Tae Heon Kim (University of Ulsan), "Polar metals by geometric design"

12:00-12:30 Ming-Wen Chu (National Taiwan University), "Emergent Charge Condensations at Two-Dimensional Oxide Interfaces"

Session SUN 3

Chair: Prof. Di-Jing Huang

14:00-14:30 Jan-Chi Yang (National Cheng Kung University), "Tuning the ferroic orders in multiferroic thin films - Role of bottom electrodes"

14:30-15:00 Tsuyoshi Kimura (Osaka University), "Multiple order parameters and their domain control in some magnetoelectric multiferroics"

15:00-15:30 Cheng-Maw Cheng (National Synchrotron Radiation Research Center (NSRRC)), "The Topologically Protected Surface State in $Sb_2Te_{3-x}Se_x$ Single Crystals with varied Se content studied by Angle-resolved Photoemission Spectroscopy"

Session SUN 4

Chair: Prof. Je-Geun Park

16:00-19:00 Poster Session I

February 20, 2017

Session MON 1

Chair: Prof. Jaejun Yu

09:00-09:30 Hidenori Takagi (The University of Tokyo/RIKEN), "Quantum Liquid state of J_{eff}=1/2 isospins"

09:30-10:00 Jae Hoon Kim (Yonsei University), "Terahertz pump-probe spectroscopy of coherent spin precession in $YMn_xFe_{1-x}O_3$"

10:00-10:30 Kenya Ohgushi (Tohoku Universtiy), "Ferroic Order of Magnetic Quadrupoles in $BaMn_2As_2$"

Session MON 2

Chair: Prof. Shik Shin

11:00-11:30 Takuro Katsufuji (Waseda University), "Photoinduced phase transitions over three phases in $AV_{13}O_{18}$"

11:30-12:00 Suyeon Cho (Ewha Womans University), "Te vacancy-driven superconducting state in Weyl semimetal $MoTe_2$"

12:00-12:30 Guang-Yu Guo (National Taiwan University), Quantum Anomalous Hall Effect in Layered Magnetic Oxides"

Session MON 3

Chair: Prof. Ying-Hao Chu

14:00-14:30 Atsushi Fujimori (The University of Tokyo), "Electronic structure of the new electron-doped cuprate superconductors in bulk and thin film forms"

14:30-15:00 Jea Hoon Park (Pohang University of Science & Technology), "Majorana Ferimons in Kitaev Quantum Spin Lattice α-$RuCl_3$"

15:00-15:30 Ashish Atma Chainani (National Synchrotron Radiation Research Center (NSRRC)), "Evidence for weakly correlated oxygen holes in the highest-Tc cuprate superconductor $HgBa_2Ca_2Cu_3O8_{+d}$"

Session MON 4

Chair: Prof. Hidenori Takagi

16:00-16:30 Yukitoshi Motome (The University of Tokyo), "Evincing Majorana fermions in Kitaev magnets"

16:30-17:00 Jaejun Yu (Seoul National University), "Possible oxygen-ordering induced ferroelectric polarization and magnetic interactions in oxygen deficient $SrCoO_{2.5+x}$"

Session TUE 1

Chair: Prof. Fu-Chun Zhang

09:00-10:00 Jan Zaanen (Leiden University), "Weak-strong duality and extremal fluctuating order"

10:00-10:30 Sang-Jin Sin (Hanyang Univ), "Holography of Dirac Fluids"

Session TUE 2

Chair: Prof. Jaejun Yu

11:00-11:30 Choong H. Kim (IBS-CCES), "Polar octahedral rotation and multiferroelectricity in the bilayer iridates"

11:30-12:00 Mehdi Biderang (APCTP), "Mixed singlet-triplet pairing and possible topological superconductivity in hole doped Sr_2IrO_4"

12:00-12:30 Wenhong Wang (Inst. of Physics, CAS), "Nonvolatile Magnetic Biskyrmion in a Centrosymmetric Hexagonal Magnet"

Session TUE 3

Chair: Prof. Shun-Qing Shen

14:00-14:30 Xi Dai (Inst. of Physics, CAS), "Heavy Weyl fermion state in $CeRu_4Sn_6$"

14:30-15:00 Shuichi Murakami (Tokyo Inst. Technology), "Symmetry and topology in topological semimetal materials"

15:00-15:30 Suk Bum Chung (IBS-CCES), "Phase Transitions and Topology in the Exciton-Polariton Condensate of the Gapped 2D Dirac Materials"

Session TUE 4

Chair: Prof. Xi Dai

16:00-16:30 Shun-Qing Shen (The Univ of Hong Kong), "Quantum Magnetotransport in Topological Semimetals"

16:30-17:00 S. A. Jafari (Sharif Univ. of Technology), "Superconducting proximity in three-dimensional Dirac materials: Majorana fermions from pseudo-scalar pairing"

17:00-17:30 Fu-Chun Zhang (Kavli Inst. for Theoretical Sciences, UCAS), "Majorana zero mode with spin selective Andreev reflection inside vortex of topological superconductor"

February 22, 2017

Session WED 1

Chair: Prof. Yunkyu Bang

09:00-09:30 Joe David Thompson (Los Alamos National Laboratory), "Quantum Criticality and Superconductivity in Heavy-Fermion Compounds"

09:30-10:00 Steffen Wirth (Max Planck Institute for Chemical Physics of Solids Dresden), "STS studies on correlated f-electron systems: the fate of the Kondo lattice"

10:00-10:30 Peter S. Riseborough (Temple Universirty), "Hidden Order in URu2Si2: A spin-dependent orbital density wave phase"

Session WED 2

Chair: Prof. Je Geun Park

11:00-11:30 Philipp Gegenwart (EP 6, Center for Electronic Correlations and Magnetism, Augsburg University), "Kitaev interaction in hexagonal iridates and rhodates"

11:30-12:00 Jonathan Denlinger (Lawrence Berkeley National Laboratory), "Progress in comparison of ARPES to DMFT for d and f strongly correlated electron systems"

12:00-12:30 Kazushi Kanoda (University of Tokyo), "Extraordinary Coulomb Correlations of Weyl fermions in an organic conductor"

Session WED 3

Chair: Prof. Kwon Park

14:00-14:30 Friedrich Malte Grosche (University of Cambridge), "Correlated states near electronic and structural instabilities"

14:30-15:00 Sung-Sik Lee (McMaster University / Perimeter Institute), "Exact critical exponents for the antiferromagnetic quantum critical metal in two dimensions"

15:00-15:30 Shuji Hasegawa (University of Tokyo), "Parity-broken monatomic-layer superconductors"

Session WED 4

Chair: Prof. Jungseek Hwang & Dr. F. Ronning & Prof. Tae-Hwan Kim

16:00-18:00 Poster Session II

Session THU 1

Chair: Prof. Changyoung Kim

09:00-09:30 Filip Ronning (Los Alamos National Laboratory), "Emergent magnetic anisotropy in cubic $CeIn_3$"

09:30-10:00 Kenji Ishida (Kyoto University), "NMR Studies on U-based Ferromagnetic Superconductors"

10:00-10:30 Ji Hoon Shim (POSTECH), "First-principles dynamical mean field theory approach on heavy fermion system"

Session THU 2

Chair: Prof. Jeajun Yu

11:00-11:30 Yeong Kwan Kim (KAIST), "What is going on in the nematic phase of iron based superconductor?"

11:00-12:00 Tetsuo Hanaguri (RIKEN CEMS), "Spectroscopic-imaging STM studies of superconductivity and nematicity in $FeSe_{1-x}S_x$"

12:20-12:30 Seung-Ho Baek (IFW-Dresden), "Spin-fluctuation-driven preformed singlet pairs in the iron-pnictide, $Na_{1-x}Li_xFeAs$"

Session THU 3

Chair: Prof. Youngjung Jo

14:00-14:30 Jun Sung Kim (POSTECH), "Ferromagnetic Van der Waals Metal Fe_3GeTe_2: from Bulk to Atomically Thin Crystals"

14:30-15:00 James G. Analytis (UC Berkeley), "Intertwinded orders in Mott-Kitaev honeycomb iridates"

15:00-15:30 Tae-Hwan Kim (POSTECH), "Switching Chiral Solitons for Algebraic Operation of Topological Quaternary Digits"

Session THU 4

Chair: Jihoon Shim

16:00-16:30 Heung-Sun Sim (KAIST), "Topological vacuum bubbles of anyons

16:30-17:00 Kenenth Stephen Burch (Boston College), Towards Topological and Unconventional Superconductivity"

February 24, 2017

Session FRI 1

Chair: Prof. Jun Sung Kim

09:00-09:30 Sang-Wook Cheong (Rutgers University), “Topologies and Emergent Phenomena of Domain walls in Quantum Materials”

09:30-10:00 Johannes Knolle (TCM Cavendish Lab, University of Cambridge), “The anomalous de Haas-van Alphen effect and Excitons in a topological Kondo insulator”

10:00-10:30 SungBin Lee (KAIST), “Symmetry enforced semimetals and symmetry enriched topologically ordered state in nonsymmorphic crystals”

Session FRI 2

Chair: Prof. Kee-Hoon Kim

11:00-11:30 Kwang-Yong Choi (Chung-Ang University), “Novel quantum states of matter and fractionalized excitations emergent in Kitaev materials”

11:30-12:00 Maria Hermanns (University of Colgone), “3D Kitaev spin liquids”

Session FRI 3

Chair: Prof. Tuson Park

12:00-12:30 Closing

Poster Session I (Feb. 19, 16:00-19:00)

Chair: Prof. Je-Geun Park

Poster I #01 Hasung Sim (Seoul National Univ.) "Doping effects on 2D triangular multiferroic $Y(Mn,Al,Ga)O_3$

Poster I #02 Joosung Oh (Seoul National Univ.), "Magnon phonon hybridization in multiferroic $RMnO_3$"

Poster I #03 Hwanbeom Cho (Seoul National Univ.), "Properties of highly frustrated antiferromagnets: $Cu\mathit{RE}_2Ge_2O_8$ RE=Pr,Nd,Sm~Tm)"

Poster I #04 Kisoo Park (Seoul National Univ.), "Low energy spin dynamics of rare-earth orthoferrites $YFeO_3$ and $LaFeO_3$"

Poster I #05 Sungmin Lee (Seoul National Univ.), "Sungmin Lee (Seoul National Univ.), "Transport study on antiferromagnetic van der Waals $MnPS_3$ using conductive atomic force microscopy"

Poster I #06 Taehun Kim (Seoul National Univ.), "Strong thermal hysteresis of Verwey transition Fe_3O_4 Nanoparticles"

Poster I #07 Seokhwan Yun (Seoul National Univ.), "Breakdown of dimerized valence bonds in $Li_2Ru_{1-x}MnxO_3$"

Poster I #08 Suhan Son (Seoul National Univ.), "Spin glass behavior in ultrathin magnetic van der Waals materials"

Poster I #09 Jonathan Leiner (Seoul National Univ.), "Spin dynamics in the spin chain compound Sr_3CuPtO_6"

Poster I #10 Arvind Yogi (Seoul National Univ.), "Evidence of electron-phonon interaction in single crystal of (Ru^{3+}/Ru^{4+}) mixed-valence $Na_{2.7}Ru_4O_9$ and $NaRu_2O_4$"

Poster I #11 Howon Lee (Yonsei Univ.), "Spin Precession Pumped by Pulsed Terahertz Magnetic Field in $YMnxFe_{1-x}O_3$"

Poster I #12 Young Chan Jo (Yonsei Univ.), "Metallic Terahertz Metamaterials Research"

Poster I #13 Donghwan Kim (POSTECH), "Effect of strong spin-orbit coupling of anion p orbitals on superexchange interaction"

Poster I #14 Junho Park (POSTECH), "Magnetic properties of epitaxially grown high quality $LaCrO_3$ films by pulsed laser deposition"

Poster I #15 Wen-Bin Wu (NSRRC), "High-Resolution Soft X-ray RIXS Using Active Gratings and Energy Compensation"

Poster I #16 Hsiao-Yu Huang (NSRRC), "Jahn-Teller distortion driven magnetic polarons in magnetite"

Poster I #17 Amol Singh (NSRRC), "Electronic structure of $Ce_3Co_4Sn_{13}$ using hard X-ray photoelectron spectroscopy & x-ray absorption spectroscopy"

Poster I #18 Yi-De Liou (National Cheng Kung Univ.), "Raman Study on Photostrictive Perovskite $SrIrO_3$ Thin Films"

Poster I #19 Ping-Chun Wu (National Chiao Tung Univ.), "Heteroepitaxy of Fe_3O_4/Muscovite: A New Perspective for Flexible Spintronics"

Poster I #20 Yen-Pei Lin (National Chiao Tung Univ.), "Van der Waals Epitaxy of Flexible and Transparent VO_2 Film on Muscovite"

Poster I #21 Min Yen (National Chiao Tung Univ.), "High Mobility Transparent Heteroepitaxy (Ba, La)SnO_3/Muscovite for Flexible Optoelectronics"

Poster I #22 Ying-Hui Hsieh (National Chiao Tung Univ.), "Creating Flexoelectrity via Composition gradient"

Poster I #23 Yosuke Nonaka (Tokyo Univ.), "Search for complex orbital order in magnetite Fe_3O_4 by magnetic-field-direction dependent XAS and XMCD measurements"

Poster I #24 Minu Kim (Max-Planck-Institute fuer Festkoerperforschung), "High-Pressure Synthesis of a Third-Family Perovskite Bismuthate"

Poster I #25 Kazuhiro Kowa (Osaka Univ.), "Structure analysis of $LaNiO_3$ /$LaAlO_3$ interface by surface X-ray diffraction"

Poster I #26 Yusuke Yoshimori (Osaka Univ.), "The pressure effect on magnetoelectricity in Cr_2O_3"

Poster I #27 Tomomasa Kajita (Waseda Univ.), "Novel relaxation behaviors in the orbital-ordered vanadates"

Poster Session II (Feb. 22, 16:00-18:00)

Chair: Prof. Jungseek Hwang & Dr. F. Ronning & Prof. Tae-Hwan Kim

Poster II #01 Sungmin Park (Sungkyunkwan Univ.), “Al doping effect on helical magnet CrAs under pressure”

Poster II #02 Sungil Kim (SungKyunKwan Univ.), “Anisotropic upper critical field in the pressure-induced superconductivity for the single crystal of CrAs”

Poster II #03 Sunghun Kim (KAIST), “Band Dependent Pseudogap Opening in Iron Pnictide Sr_2VO_3FeAs”

Poster II #04 Jong Mok Ok (POSTECH), “Multiple Fulde-Ferrel-Larkin-Ovchinnikov states in FeSe”

Poster II #05 Jong Mok Ok (POSTECH), “Emergent electronic phases in a hetero-structured iron-based superconductor”

Poster II #06 Chan Hee Kim (Seoul National Univ.), “Evidence of nodeless multigap superconductivity in 2H-Pd_xTaSe_2 from London penetration depth and thermal transport”

Poster II #07 Min-Cheol Lee (IBS-CCES), "Non-equilibrium lattice vibrations of As ions in spin-density-wave state of $BaFe_2As_2$"

Poster II #08 Seokbae Lee (Sungkyunkwan Univ.), “Hidden non-Fermi liquid properties of $BaFe_{2-x}NixAs_2$ pnictides”

Poster II #09 Yea Han Sur (Seoul National Univ.), “Hydrostatic Pressure Effects on the Superconductivity of $Ca_{0.9}La_{0.1}FeAs_2$ Single Crystal”

Poster II #10 DILIP KUMAR BHOI (Seoul National Univ.), “Interplay of charge density wave and multiband superconductivity in 2H-Pd_xTaSe_2”

Poster II #11 Canceled

Poster II #12 Soon-Gil Jung (Sungkyunkwan Univ.), “Observation of quantum critical point by pressure evolution of critical current density in $CeRhIn_5$”

Poster II #13 Soonbeom Seo (SungKyunKwan Univ.), “Pinned Quantum Critical Point in the Hg doped $CeRhIn_5$”

Poster II #14 Sangyun Lee (SungKyunkwan Univ.), “Pressure-induced Superconducting State in $MoTe_2$”

Poster II #15 JinKwon Kim (IBS CCES, SNU), “Strain dependence of superconducting $BaPb_{1-x}Bi_xO_3$ thin film”

Poster Session II (Feb. 22, 16:00-18:00)

Poster II #16 Woo Hyun Nam (Seoul National Univ.), "Suppression of Tc and magnetic impurity effects in the single crystals of $Li(Fe_{1-x}Mn_x)As$"

Poster II #17 Chan Koo Park (SungKyunkwan Univ.), “Synthesis and characterization of the Ce doped $LaIn_3$”

Poster II #18 Byungcheol Park (IBS-CCES), “Ultrafast Terahertz Dynamics of $Ba_{0.6}K_{0.4}BiO_3$ Superconducting Thin Films”

Poster II #19 AGA SHAHEE (Seoul National Univ.), “Development of low temperature and high magnetic field Powder X-ray diffraction facility for field-driven structural”

Poster II #20 Taesik Nam (POSTECH), “Electronic structures of Ce-based Kondo insulators”

Poster II #21 Bumjoo Lee (IBS-CCES), “Ultrafast study of topological insulator Bi_2Te_3 single crystal”

Poster II #22 Junyeong Ahn (Seoul National Univ.), “Unconventional topological phase transition in two-dimensional systems with space-time inversion symmetry”

Poster II #23 Sungjoon Park (Seoul National Univ.), “Classification of gap closing process through band inversion in layer groups”

Poster II #24 Chang Bae Park (Seoul National Univ.), “Measurement of size dependent magnetoelectric coupling in Fe_3O_4 nanoparticles”

Poster II #25 SoonHee Park (GIST), “Pressure-induced insulator-metal transition in $Ca_2Ru_{0.92}Fe_{0.08}O_4$ investigated by infrared microspectroscopy”

Poster II #26 Bo Gyu Jang (POSTECH), “Role of Correlation Effect on O_2 dimer bond length and Metal-Insulator Transition of FeO_2”

Poster II #27 Inho Kwak (IBS-CCES), “Ultrafast study on metal-insulator transition in 5d pyrochlore $Cd_2Os_2O_7$”

Poster II #28 Jeong Hyuk Lee (Seoul National Univ.), "Transparent p-CuI/n-BaSnO3-δ Wide Bandgap Heterojunction Diodes"

Poster II #29 Shoresh Soltani (IBS-CCES, Yonsei Univ.), “Angle resolved photoemission spectroscopy studies on the surfaces of $SrTiO_3$ and $KTaO_3$”

Poster II #30 Hoil Kim (POSTECH), “Berry phase crossover in a Nodal Line Semimetal $SrAs_3$”

Poster II #31 Alexey Andreanov (IBS PCS), “Compact localized states and flatband generators in one dimension”

Poster Session II (Feb. 22, 16:00-18:00)

Poster II #32 JungHyun Seo (Hanyang Univ.), "Doping and temperature dependence of the electronic structure of $(Sr_{1-x}La_x)_2IrO_4$"

Poster II #33 Jae-Hoon Sim (KAIST), "Dynamical mean-field theory of $LaTiO_3$ /$LaAlO_3$ superlattice"

Poster II #34 InHyeok Choi (GIST), "Dynamics of single- and multi-vertical-Bloch-line in canted antiferromagnetic rare-earth orthoferrites"

Poster II #35 Archana Mishra (KAIST), "Effect of interactions in the Hofstadter regime of the honeycomb lattice"

Poster II #36 So Yeun Kim (Seoul National Univ.), "Electronic structure study on magnetic vdW material $NiPS_3$"

Poster II #37 Taekoo Oh (Seoul National Univ.), "Emergent topological phases in pyrochlore iridates under magnetic field"

Poster II #38 GiBaik Sim (KAIST), "Generic spin model on a pyrochlore lattice"

Poster II #39 Canceled

Poster II #40 Muhammad Nauman (Kyungpook National Univ.), "Magnetic Anisotropies in Iridates"

Poster II #41 Seulki Roh (Sungkyunkwan Univ.), "Polarized optical spectroscopy on anisotropic $BaFe_2Se_3$ single crystal"

Poster II #42 Jaeseok Son (IBS-CCES), "Strong spin-phonon coupling behavior in All-In/All-Out Pyrochlore iridates $R_2Ir_2O_7$ (R = Y, Eu, Sm)"

Poster II #43 Jongkeun Jung (Seoul National Univ.), "Study of CO oxidation activity on the bimetallic $Pt_3Sn(111)$ surfaces by ARPES"

Poster II #44 Soohyeon Shin (SungKyunKwan Univ.), "Synthesis and Characterization of the Heavy-Fermion Compound $CePtAl_4Ge_2$"

Poster II #45 Ha Rim Jang (SungKyunKwan Univ.), "Synthesis and Thermal Annealing effects on $BaFe_{2-\delta}Se_3$"

Poster II #46 Hanyoung Ryu (IBS-CCES. SNU), "Photon energy dependent circular dichroism in angle-resolved photoemission from Au(111) surface state"

Poster II #47 Kyongjun Yoo (Seoul National Univ.), "Observation of magnetoelectric effects in $PbCu_3TeO_7$"

Poster II #48 Garam Han (IBS-CCES. SNU), "Crystal and electronic structure studies on Bandwidth controlled Mott transition in $NiS_{2-x}Se_x$"

Electron Spin Resonance of single atoms on a surface

Andreas Heinrich[12]

[1] *Center for Quantum Nanoscience, Institute of Basic Science, Seoul, South Korea*
[2] *Physics Department, Ewha Womans University, Seoul, South Korea*

The scanning tunneling microscope is an amazing experimental tool because of its atomic-scale spatial resolution. This can be combined with the use of low temperatures, culminating in precise atom manipulation and spectroscopy with microvolt energy resolution. In this talk I will apply these techniques to the investigation of the quantum spin properties of transition metal atoms on surfaces. We will conclude with our recent measurements of electron spin resonance in an STM on individual Fe atoms supported on an insulating thin film, offering unprecedented energy resolution on the atomic scale. This tool can be used as an ESR sensor to measure the magnetic field (dipolar interaction) from neighboring atoms, enabling the high-precision measurement of the magnetic moment of individual atoms on surfaces.

Oral Sun1-02

Laser-PEEM study on the photo-induced ferromagnetism in $SrTiO_3$ surface

Shik Shin[1]

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

We report the first experiments carried out on a new chemical and magnetic imaging system, which combines the high spatial resolution of a photoemission electron microscopy (PEEM) with a continuous wave (CW) deep ultraviolet laser. We achieved the spatial resolution of 2.6 nm [1]. This is the highest resolution of the world as the PEEM.

We would like to report the ferromagnetic domain structures of two-dimensional-electron-gas on $SrTiO_3$ perovskite oxide surfaces [2]. We will also report the photo-induced ferromagnetism on Sc-doped $SrTiO_3$.

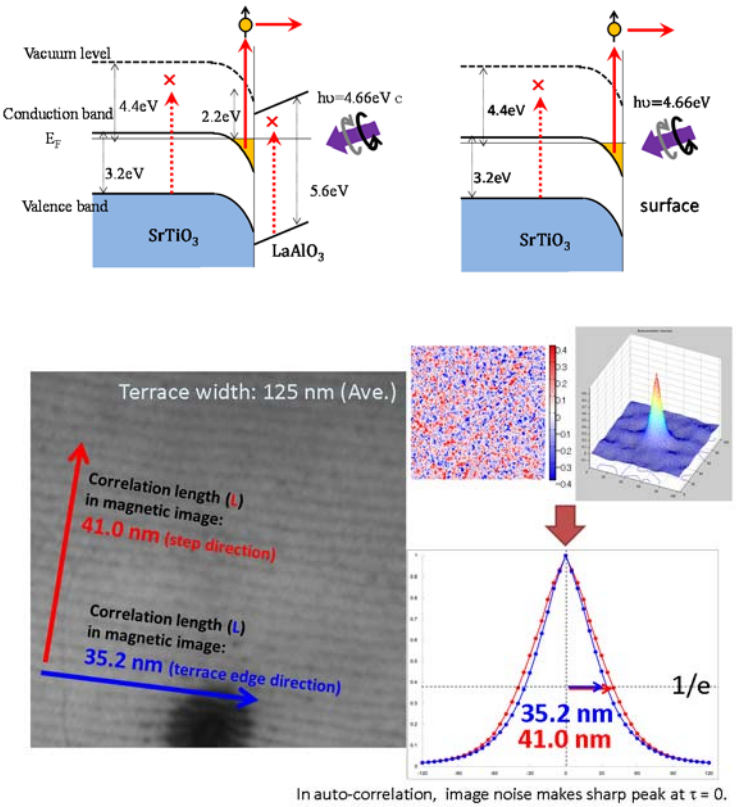

Fig.1 Feromagnetic domain structures of $SrTiO_3$ surface[2]

[1] T.Taniuchi, Y.Kotani, S.Shin, Rev. Sci. Instrum.**86**, 023701 (2015)

[2] T.Taniuchi, Y.Motoyui, K.Morozumi, T.C.Rödel, F.Fortuna, A.F.Santander-Syro, S. Shin, Nature Commun.7, 11781(2016)

Spin crossover of cobaltates revealed by resonant inelastic X-ray scattering

Di-Jing Huang[1]

[1]*National Synchrotron Radiation Research Center, Hsinchu 30076, TAIWAN,*
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Spin-state transitions or crossovers between low-spin and high-spin states occur in diverse materials. While the preferred model of thermal evolution is based on changes in the crystal-field excitations of transition-metal ions, the associated changes in Coulomb energies across spin-state transitions are not known from experiment. Here we demonstrate that resonant inelastic X-ray scattering (RIXS) effectively characterizes the evolutions of the high and low spin states in LaCoO3, respectively, when the temperature is changed across the spin crossover temperature. Markedly the results indicate that one can use a high-energy (~1.3 eV) excitation method to unravel a spin-state transition which is triggered by a temperature change equivalent to an energy change less than 10 meV. The RIXS approach establishes a new window to understanding the spin sate
transition of transition metal compounds, particularly those containing transition metal ions with a $3d^6$ electronic configuration.

This work was done in collaboration with K. Tomiyasu, J. Okamoto, H. Y. Huang, Z. Y. Chen, E. P. Sinaga, W. B. Wu, Y. Y. Chu, A. Singh, R.-P. Wang, F. M. F. de Groot, C. T. Chen, A. Chainani, and S. Ishihara.

Oral Sun2-01

Flexible Oxide Heteroepitaxy: A New Playground for Exploring Intriguing Properties of Functional Oxides

Ying-Hao Chu[1,2,3,4]

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[2] *Department of Electrophysics, National Chiao Tung University, Hsinchu 30010, Taiwan*
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In the diligent pursuit of low-power consumption, multifunctional, and environmentally friendly electronics, more sophisticated requirements on functional materials are on demand. For example, flexible electronics represents a fast-developing field and has a great potential to impact our daily life. In building up flexible electronics, the materials with controllable conduction, transparency, and good flexibility are required. Recently, the discovery of free-standing 2D materials has created a revolution to this field. Pioneered by graphene, these new 2D materials exhibit aboundant unusual physical phenomena that is undiscovered in bulk forms. In the meantime, it also possesses very high transparency to the visible light. However, the extensively studied pristine graphene naturally has no bandgap and become restricted in many field-effect based applications. Hence, looking for various types of new 2D materials has been a focal research direction nowadays. In this talk, we intend to take the same concept, but to integrate a family of functional materials in order to open new avenue to flexible electronics. Due to the interplay of lattice, charge, orbital, and spin degrees of freedom, correlated electrons in oxides generate a rich spectrum of competing phases and physical properties. However, a generic approach to build up flexible electronics based on functional oxides is yet to be developed. In this study, we use a 2D material as the substrate. And we take several functional oxides as a models system to demonstrate a pathway to build up functional oxides for transparent and flexible electronics.

Polar metals by geometric design

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In general, metallic conductivity and polar displacements are not compatible each other, because free electrons in a metal effectively screen electric dipoles. Despite the incompatibility, 'polar metals', where itinerant electrons and electric dipole moments coexist, have been discovered in various material systems for several decades, offering the potential for novel device applications [1,2]. In contrast with these exciting findings of exotic polar metallic states, a feasible approach for realization of the polar metals has never been provided, yet.

A key to design polar metal is that electronic conduction is structurally decoupled from polar displacements. In ternary perovskite ABO_3 oxides, the multiple A and B cations provide two sublattices, which allow one to contribute partially-occupied delocalized states for conduction, while the other is able to undergo polar distortion in response to changes in the BO_6 octahedra. For this aim, we selected strongly-correlated rare-nickelates RNiO$_3$, which undergo a thermally-driven metal-to-insulator transition depending on the crystallographic tolerance factor [3]. Among them, $NdNiO_3$ is a suitable candidate, which is electronically conductive at room temperature and structurally orthorhombic (*Pnma*) due to the tilting of NiO_6 octahedra. Note that A-site polar displacements with respect to oxygen atoms can be attained in perovskite oxides, when the tilting of BO_6 octahedra is suppressed [4]. Thus, by achieving a non-equilibrium tilt pattern of NiO_6 octahedra, we could realize a polar metallic state in $NdNiO_3$, where finite band occupancy of Ni 3*d* orbitals for metallicity and an acentric Nd-oxygen displacement coexist.

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Emergent Charge Condensations at Two-Dimensional Oxide Interfaces

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With the assistance of modern thin-film growth techniques, perovskite oxides with a three-dimensional crystal structure can now be grown in a layer-by-layer manner at atomic-level precision on heterostructural substrates, opening up vast opportunities for unprecedented phenomena at the two-dimensional (2D) oxide interfaces. The emergence of a conductive interface between the two band insulators, $LaAlO_3$ (LAO) and $SrTiO_3$ (STO), represents the most celebrated exemplification in this context. Up to the date, a plethora of unexpected properties have been established at oxide heterointerfaces, ranging from 2D electron gas, 2D superconductivity, 2D orbital reconstruction to 2D magnetic ordering. However, why can be the oxide interfaces so surprising? This remains an outstanding unresolved problem. This speaker intends to elucidate on how to tackle the puzzle using atomic-plane-by-atomic-plane and unit-cell-by-unit-cell scrutiny of charge, lattice, and electronic-structure degrees of freedom in interfacial unit cells by atomically-resolved electron spectroscopy. Several intriguing phenomena were readily resolved, including the presence of localized 2D electron density at the insulating (Nd,Sr)MnO_3/STO interface [C.-P. Chang *et al.*, Phys. Rev. B **87**, 075129 (2013)], the condensation of the 2D interfacial charges in (Nd,Sr)MnO_3/STO into one-dimensional electron chains by the misfit-dislocation strain field [C.-P. Chang *et al.*, Nat. Commun. **5**, 3522 (2014)], and the hidden lattice instabilities as the origin of the conductive LAO/STO interface [P. W. Lee *et al.*, Nat. Commun. **7**, 12773 (2016)]. Perspectives on 2D oxide-interfacial phenomena will also be discussed.

Tuning the ferroic orders in multiferroic thin films - Role of bottom electrodes

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The strong coupling between (anti)ferromagnetism and ferroelectricity found in multiferroics has triggered high expectations for the development and design of technological devices with multifunctionalities. Researchers have been enthusiastically devoted to the development of effective modulation on these intriguing coupling and phenomena among multiferroics via external stimuli. Due to the correlations between intrinsic degrees of freedom, the electrical and magnetic field are usually the most conventional ways to reach external control on the correlated phenomena. In order to enrich the tunability, the exploration of additional factors or controlling parameters to modulate the lattice, charge, orbital, and spin degrees of freedom in multiferroics has received more and more demand to cooperate with the existing approaches.

In this talk, we will spin on the intriguing role played by functional bottom electrodes, in terms of tuning ferroic orders in room temperature multiferroic $BiFeO_3$. The insertion of bottom electrodes not only could be used to stabilize single domain feature in $BiFeO_3$ thin films, but also enables the thin films being tuned via new controlling factor, light. Through a combination of x-ray diffraction, piezoforce microscopy and x-ray absorption spectroscopy, we found free charges in bottom electrode that have the opposite sign to the surface charges of ferroelectric would like to approach ferroelectric-electrode interface, resulting in a 'built-in electric field' for stabilization single domain multiferroic $BiFeO_3$ films. More importantly, the incorporation of bottom electrode that shows significant photostriction has endowed the ferroic orders in $BiFeO_3$ with new tunabilities driven by light illumination. Such results offer a new pathway to control the intriguing physical properties through the correlations between ferroic orders and external stimuli, which lead to new-generation multifunctional applications.

Oral Sun3-02

Multiple order parameters and their domain control in some magnetoelectric multiferroics

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One of the most important concepts in condensed matter physics is the spontaneous breakdown of symmetry in a solid, which bears the ordered phase and domains in its consequence. In magnetoelectric multiferroics, multiple order parameters coexist in a system, sometimes couple with each other, and exhibit nontrivial crossed phenomena. In this presentation, we deal with magnetoelectric multiferroics in which a symmetry breaking due to the orderings of various order parameters such as electric dipole, magnetic dipole, and magnetic quadrupole moments as well as chirality originating from these multipole moments. We show our recent research activity on exploration for new magnetoelectrics and manipulations of their multiple order parameters as well as domains.

This work has been done in collaboration with K. Kimura, H. Ueda, M. Sera, T. Honda, T. Aoyama, Y. Wakabayashi, K. Yamauchi, M. Toyoda, K. Shimizu, Y. Tanaka, P. Babkevich, H. M. Rønnow, J. S. White, M. Kenzelmann et al.

The Topologically Protected Surface State in $Sb_2Te_{3-x}Se_x$ Single Crystals with varied Se content studied by Angle-resolved Photoemission Spectroscopy

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A topological insulator (TI) is a new class of quantum material with attractive properties for physical and technological applications. Regarding topological insulators (TI) in the bismuth family, most work has focused on Bi_2Se_3, Bi_2Te_3 and $Bi_2Se_{3-x}Te_x$ compounds, but experimental work on *p*-type $Sb_2Te_{3-x}Se_x$ ternary topological insulators is lacking. Here we derive the electronic structure of highly crystalline $Sb_2Te_{3-x}Se_x$ single crystals with varied Se content studied with angle-resolved photoemission spectra. The result of band mapping reveals that the $Sb_2Te_{3-x}Se_x$ compounds with x=2.4 still behave as a *p*-type semiconductor and have an isolated Dirac cone of a topological surface state, which are highly favored for spintronic and thermoelectric devices because of the dissipationless surface state and the decreased scattering from bulk bands. More importantly, a Sb bilayer (BL) was successfully grown on Sb_2Te_3 single crystal, we found that the position of the Dirac point almost located at the Fermi level. The band hybridization of Sb/Sb_2Te_3 in band gap engineering makes a potential to fabricate a spintronic devices in the future.

Oral Mon1-01

Quantum Liquid state of J_{eff}=1/2 isospins

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In 5d Iridium oxides, the relativistic spin-orbit coupling for 5d electrons is as large as ~0.5 eV and not small as compared with other relevant electronic parameters, including Coulomb U, transfer t and crystal field splitting D. The large spin-orbit coupling and its interplay with the other parameters gives rise to a variety of exotic magnetic ground states. In the layered perovskite Sr_2IrO_4, spin-orbital Mott state with J_{eff}=1/2 is realized due to the novel interplay of those energy scales [1]. Despite the strong entanglement of spin and orbital degrees of freedom, J_{eff}=1/2 iso-spins in Sr_2IrO_4 was found to be surprisingly isotropic, very likely due to a super-exchange coupling through almost 180° Ir-O-Ir bonds [2]. The temperature dependence of in-plane magnetic correlation length of J_{eff}=1/2 iso-spins, obtained from inelastic x-ray resonant magnetic scattering, was indeed well described by that expected for two-dimensional S=1/2 Heisenberg antiferromagnet [3].

When J_{eff}=1/2 iso-spins interact with each other through 90° Ir-O_2-Ir bonds, an Ising ferromagnetic coupling with an easy axis perpendicular to the bond plane is expected, due to an interference of the two Ir-O-Ir superexchange paths [2]. In α, β,γ-Li_2IrO_3 with honeycomb based structure, J_{eff}=1/2 iso-spin are connected by the three competeting 90° Ir-O_2-Ir bonds, which could be a materialization of Kiatev model [4] with quantum spin liquid state. A long range magnetic ordering, however, was observed at low temperatures in α, β,γ-Li_2IrO_3, which is very likely due to the presence of additional magnetic couplings not included in the original Kitaev model [4]. The exploration of Kitaev state was recently extended to related compounds and pressure effect. We found that a quantum spin liquid state is realized in hydorogenated Ir 2D honeycomb (α-type) and β-Li_2IrO_3 under high pressure [5]. The search for possible fractionalized excitations, expected for Kitaev spin liquid, is now underway.

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Terahertz pump-probe spectroscopy of coherent spin precession in $YMn_xFe_{1-x}O_3$

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We report on our recent study of coherent spin dynamics in canted antiferromagnetic $YMn_xFe_{1-x}O_3$ (x=0-0.45) based on terahertz-pump terahertz-probe spectroscopy. Both the quasi-ferromagnetic resonance mode (qFMR) and the quasi-antiferromagnetic resonance mode (qAFMR) were detected. We can probe a number of distinct magnetically ordered phases by varying temperature and Mn doping. Spin reorientation transition and new infrared-active resonance modes were also observed.

Oral Mon1-03

Ferroic Order of Magnetic Quadrupoles in $BaMn_2As_2$

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Kondo effect is one of the most fascinating phenomena in condensed matters. The phenomenon is realized when conduction electrons couple with a localized spin; the spin is an even-parity magnetic dipole moment. A natural extension of this phenomenon is a quantum transport in a system, in which conduction electrons couple with a higher order electric or magnetic multipole. Among higher-order multipoles, we are particularly interested in odd-parity multipoles such as electric octupole and magnetic quadrupole. When odd-parity multipoles are ordered in a ferroic manner, one can expect a novel quantum transport induced by the breakdown of inversion symmetry.
Up to now, we have found some novel materials, in which odd-parity multipoles are ordered in a ferroic manner. Examples include $A_2Re_2O_7$ (A = Cd and Pb) and $Pb_2Ir_2O_7$ with the electric octupole order [1, 2]. In this presentation, I will introduce our recent research, which identifies a novel ferroic order of magnetic quadrupoles in $BaMn_2As_2$.

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Photoinduced phase transitions over three phases in $AV_{13}O_{18}$

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$Ba_{1-x}Sr_xV_{13}O_{18}$ with V ions on a quasi-fcc lattice exhibits two different ordered phases, a V-trimer phase with orbital ordering [low-temperature (LT) phase)] and a charge-ordered phase [intermediate-temperature (IT) phase], in addition to a high-temperature (HT) phase. We performed a pump-probe spectroscopy measurement of this compound and found that when a laser pulse is applied to the LT phase, successive phase transitions over the three phases, an instantaneous ($t << 0.5$ ps) transition from the LT phase to the HT phase, followed by a transition within 2 ps to the IT phase, occur. These photoinduced successive phase transitions are dominated by the symmetry of the three phases; both the LT phase and the IT phase are a subgroup of the HT phase but there is no such relationship between the LT phase and the IT phase. Namely, the phase transition from the LT to the HT phase is directly caused by photoexcited electrons, whereas the transition to the IT phase occurs only after the temperature of the lattice is increased by the photoirradiation.

Oral Mon2-02

Te vacancy-driven superconducting state in Weyl semimetal $MoTe_2$

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Two-dimensional (2D) transition metal dichalcogenides (TMDs) have enriched condensed matter physics, provoking the discovery of diverse quantum electronic states such as topological insulating (TI), Weyl semimetallic (WSM) and superconducting states. The superconductivity under the high pressure or the ionic gating in group 6 TMDs becomes one of the central issues because of competition with their predicted WSM states. However, the diversity in crystal structures and the complexity of phase transitions have hindered the rigorous study on the relation between superconducting and WSM states. In this study, we found the emergence of superconductivity in Te-deficient $MoTe_{2-x}$ while stoichiometric $MoTe_2$ shows no superconducting state, but exhibits a large magnetoresistance originating from its bipolar nature. Scanning tunnelling spectroscopy and synchrotron X-ray diffraction combined with theoretical calculations clarify that Te vacancies trigger superconductivity via intrinsic electron doping. This chalcogen vacancy-induced superconductivity provides a new route for cultivating superconductivity and rich electronic states, such as WSM and TI states, in TMDs and other 2D van der Waals materials.

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Quantum Anomalous Hall Effect in Layered Magnetic Oxides

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Quantum anomalous Hall (QAH) phase is a two-dimensional bulk ferromagnetic insulator with a nonzero Chern number usually in presence of spin-orbit coupling (SOC). Associated metallic chiral edge states carry dissipationless current transport in electronic devices. Due to its intriguing nontrivial topological properties and great potential application for designing dissipationless spintronics, extensive theoretical and experimental studies have been made to search for real materials to host such QAH effect. Indeed, this intriguing QAH phase has recently been observed in magnetic impurity-doped topological insulators at extremely low temperatures (~30 mK) [1]. Based on first-principles density functional calculations, we predict that the QAH phases would exist in two kinds of layered 4d and 5d transition metal oxides with honeycomb and triangular lattices at high temperatures [2-3]. Furthermore, theoretical analysis reveals that the QAH phases in these oxide systems originate from two distinctly different mechanisms [2-3], namely, the conventional one due to the presence of both the SOC and ferromagnetism in the $(LaAlO_3)_{10}/(LaOsO_3)_2$ perovskite superlattice along the [111] direction [2], and the unconventional one (quantum topological Hall effect) caused by nonzero spin chirality resulting from topologically nontrivial magnetic structure in noncoplanar antiferromagnetic oxide $K_{0.5}RhO_2$ [3].

The speaker acknowledges that the works presented here were carried out in collaboration mainly with Hirak Kumar Chandra, Jian Zhou and Qi-Feng Liang.

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Oral Mon3-01

Electronic structure of the new electron-doped cuprate superconductors in bulk and thin film forms

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In the electron-doped cuprates with the T' structure, superconductivity appears only after reduction annealing in the Ce-doping range of $0.13 < x < 0.18$ for $Nd_{2-x}Ce_xCuO_4$, and strong antiferromagnetic (AFM) correlation persists even in the superconducting phase. Recently, thin films of R_2CuO_4 (R = Nd, Pr) without Ce doping [1] and bulk crystals of $Pr_{1.3-x}La_{0.7}Ce_xCuO_4$ with Ce doping as low as $x \sim 0.05$ [2] have shown superconductivity after special annealing treatment.

We have performed systematic studies of the new T'-type cuprates superconductors in bulk and thin film forms by ARPES [3], x-ray photoemission spectroscopy, and x-ray absorption spectroscopy. By the reduction annealing, the signature of AFM correlation disappeared, the electron carrier concentration increased, and the Tc increased, in particular in samples with lower Ce content. The amount of increase in carrier concentration indicates that not only apical oxygen atoms but also in-plane and/or block-layer oxygen atoms are removed by annealing.

This work has been done in collaboration with M. Horio, K. Okazaki, T. Mizokawa, T. Yoshida, A. Ino, H. Anzai, M. Arita, H. Namatame, M. Taniguchi, S. Shin, Y. Ohta, H. Wadati, S. Shin, M. Kobayashi, K. Horiba, H. Kumigashira, Y. Krockenberger, H. Yamamoto, T. Adachi, and Y. Koike.

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Majorana Ferimons in Kitaev Quantum Spin Lattice α-$RuCl_3$

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Geometrical constraint often enforces the electronic states of matter to be topological quantum states such as fractional quantum Hall states, topological insulators, and Weyl semi-metals. In magnetism, theoretical studies predicted an entangled magnetic quantum state with topological ordering and fractionalized spin excitations, the so-called quantum spin liquid (QSL). The Kitaev honeycomb lattice is envisioned as an ideal host for Majorana fermions (MFs), fractionalized spin excitations created out of QSL. Here I will discuss thermally fractionalized Majornara fermions in Kitaev quantum spin lattice a-$RuCl_3$.

Oral Mon3-03

Evidence for weakly correlated oxygen holes in the highest-T_c cuprate superconductor $HgBa_2Ca_2Cu_3O_{8+\delta}$

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We study the electronic structure of $HgBa_2Ca_2Cu_3O_{8+\delta}$ (Hg1223 ; T_c = 134 K), the highest-T_c cuprate superconductor at ambient pressure, using photoemission spectroscopy (PES) and x-ray absorption spectroscopy (XAS). Resonant valence band PES across the O K-edge and Cu L-edge identify correlation satellites originating in O 2p and Cu 3d two-hole final states, respectively. Analyses using the experimental O 2p and Cu 3d partial density of states show quantitatively different on-site Coulomb energies for the Cu-site (U_{dd} = 6.5 eV $\pm$ 0.5 eV) compared to the O-site (U_{pp} = 1.0 eV $\pm$ 0.5 eV). Cu_2O_7-cluster calculations with non-local screening explain the Cu 2p core level PES and Cu L-edge XAS spectra, confirm the U_{dd} and U_{pp} values, and provide evidence for the Zhang-Rice singlet state in Hg1223. In contrast to known results on other hole-doped cuprates and 3d-transition metal oxides, the present results indicate weakly correlated oxygen holes in Hg1223.

*Work done in collaboration with M. Sicot, Y. Fagot-Revurat, G. Vasseur, J. Granet, B. Kierren, L. Moreau, D. Malterre *(Institut Jean Lamour, Université de Lorraine, Nancy, France)* ; M. Oura *(RIKEN SPring-8 Centre, Hyogo 679-5148, Japan)* ; A. Yamamoto, Y. Tokura, *(Strong Correlation Physics Division, RIKEN Center for Emergent Matter Science (CEMS), Wako 351-0198, Japan)*.

Evincing Majorana fermions in Kitaev magnets

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After the inspiring proposal by P. W. Anderson in 1973, the quantum spin liquid (QSL) has attracted continuous interest as a new quantum state of matter in magnets. Although several candidate materials have been synthesized, it remains elusive to prove that their low-temperature state is a QSL, mainly because of the lack of conventional order parameters within the Landau-Ginzburg-Wilson theory. On the other hand, one of the salient features of QSLs is the fractionalization of quantum spins associated with the topological order, which may provide a key to identify QSLs. We address this issue in the Kitaev model and its extensions, in which the quantum spin fractionalizes into two types of Majorana fermions in the QSL ground state. By using the newly-developed simulation techniques in the Majorana fermion representation, we find that the paramagnetic state harboring the QSL indicates the signatures of Majorana fermions in the temperature and energy dependences of many experimentally accessible quantities, such as the specific heat, entropy, magnetic susceptibility, dynamical spin structure factor, NMR relaxation rate, Raman scattering intensity, and thermal conductivity. Our findings will be helpful as 'smoking gun' experiments for QSLs. We discuss our theoretical results in comparison with the available experimental data for several Kitaev candidate materials.

This work has been done in the collaborations with Joji Nasu, Junki Yoshitake, Masafumi Udagawa, Yasuyuki Kato, Yoshitomo Kamiya, Johannes Knolle, Dmitry Kovrizhin, and Roderich Moessner. This research has been supported by JSPS KAKENHI Grant Numbers JP15K13533, JP16K17747, and JP16H02206. Parts of the numerical calculations are performed in the supercomputing systems in ISSP, the University of Tokyo.
References will be found in http://www.motome-lab.t.u-tokyo.ac.jp/publication-e.html.

Possible oxygen-ordering induced ferroelectric polarization and magnetic interactions in oxygen deficient $SrCoO_{2.5+x}$

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Layered $SrCoO_{2.5+x}$, a family of non-stoichiometric perovskites, has been reported to undergo topotactic ion exchange and intercalation reactions. Its property is expected to be useful for technology applications involving oxygen ion transport, such as solid oxide fuel cells and electrochemical sensors. We investigate the electronic structure and magnetic properties of the antiferromagnetically ordered $SrCoO_{2.5}$ with brownmillerite-type structure and the ferromagnetic $SrCoO_3$ with cubic-type perovskite structure by using first-principles electronic structure calculations. The relaxed structure of $SrCoO_{2.5}$ is compared with the experimental structure. The magnetic and orbital orderings related to the structural feature are observed in each layer, where the ordering of oxygen tetrahedra in $SrCoO_{2.5}$ attributed to the ferroelectric moment observed in similar brownmillerite compounds. The magnetic exchange interaction parameters between nearest-neighbor Co ions are obtained through fitting the total energy results to the model hamiltonians, and the results are found to be consistent with the observed magnetic structures of $SrCoO_3$ and $SrCoO_{2.5}$. A magnetic and structural configuration for the $SrCoO_{2.75}$ oxygen deficient structure is suggested from the results of electronic structure calculations. This finding provides us a way to understand how the electronic and magnetic ground states of $SrCoO_{3-x}$ vary depending on the amount of oxygen vacancies.

Weak-strong duality and extremal fluctuating order

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Due to exciting developments both on the computational- and experimental frontiers the 1990's theme of "fluctuating stripes" is presently reviving. Thus refers to the possibility that the superconducting quantum liquids realized in underdoped cuprates could be characterized by very strong "crystalline" (or "charge order") correlations. The conventional theoretical treatment of superconductors departs from the *uncorrelated* quantum gas limit (BCS, Bogoliubov theory). Mobilizing a big gun of quantum field theory (weak-strong duality) it appears possible to formulate a very powerful and precise mathematical theory describing bosons ("preformed pairs") forming a superconductor that is characterized by the *maximal* degree of crystalline correlations [1]. It is particularly natural to use this theory to describe the physics of superconducting quantum liquid crystals [2]. It is surprisingly easy to compute the universal physics realized in this limit and a little universe of new phenomena shows up. The phonons of the crystal turn into "stress photons", propagating elastic forces much in the same way as the usual photons propagate electromagnetic forces. In the superconducting liquid the shear forces "acquire a Higgs mass" and the transversal phonons survive as "massive shear photons". The rotational Goldstone bosons of the nematic [2] superconductor are confined in the crystal in a striking analogy with confinement in QCD. In smectic superconductors the translational-, rotational and superfluid rigidities form a "intertwined wholeness" of a new kind, to name a few. As always in physics, although reality is usually in the middle, it is very useful to know the limits and anybody who is interested in "fluctuating order" should study this theory of the maximally correlated limit.

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Oral Tue1-02

Holography of Dirac Fluids

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Recent experiments have uncovered evidence of the strongly coupled nature of graphene: the Wiedemann-Franz law is violated by up to a factor of 20 near the charge neutral point. We describe this strongly coupled plasma by a holographic model in which there are two distinct conserved U(1) currents. We find that our analytic results for the transport coefficients for the two current model have a significantly improved match to the density dependence of the experimental data than the models with only one current. The additive structure in the transport coefficients plays an important role. We also suggest the origin of the two currents. If time allows, I will talk about the magneto-conductiance at surfaces of Topological insulators.

Polar octahedral rotation and multiferroelectricity in the bilayer iridates

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Most perovskite oxides undergo octahedral rotation which strongly influence other electronic, magnetic, and orbital degree of freedom in perovskites and related materials. Hybrid improper ferroelectricity is described by trilinear coupling of two types of octahedral rotation in A-site ordered perovskites or n=2 Runddlesden-Popper structures. Polar octahedral rotation consequently have the potential to realize new multifunctional materials with strong magnetoelectric coupling. Here we propose and demonstrate hybrid improper ferroelectricity appearing in bilayer perovskite iridates $Ca_{3-x}Sr_xIr_2O_7$ from first-principles density-functional-theory calculations. Its similarity to parent compound cuprates of high-temperature superconductor makes iridates a good candidate for exploring unconventional superconductivity upon carrier doping. And *d*-wave charge gap by electron doping was observed by several experiments. In this regards, controllability of magnetism could provide a new opportunities to study superconductivity. Our proposal provide novel route to control magnetism via polar octahedral rotation.

Oral Tue2-02

Mixed singlet-triplet pairing and possible topological superconductivity in hole doped Sr_2IrO_4

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We investigate the potential existence of a superconducting phase in hole doped Sr_2IrO_4, as an example of the new class of Mott insulators. Currently, remarkable attentions have been attracted to exotic physics driven by the interplay of spin-orbit coupling and electronic correlations. Particularly, in 5d transition metals neither the spin-orbit coupling nor the Coulomb interaction can merely lead to the insulating behaviour. A very interesting question is whether these materials with very similar properties to cuprates can clarify the essential microscopic physics of High T_c superconductivity? To answer to this question, using a mean field approach we find a mixed singlet-triplet superconductivity due to antisymmetric exchange originating from a quasi-spin-orbit-coupling in hole doped Sr_2IrO_4. Our calculation on ribbon geometry shows possible existence of the topologically protected edge states while the spin-triplet component of order parameter is larger than the spin-singlet one. These edge modes emerge as zero energy flat bands and host Majorana fermions obeying non-Abelian statistics. We propose an innovative approach for experimental observation of these edge states based on the quasi-particle interference (QPI) technique.

Nonvolatile Magnetic Biskyrmion in a Centrosymmetric Hexagonal Magnet

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Magnetic skyrmion nanodomains are presently attracting immense research interest on the global level as they are arguably the smallest spin textures in nature and thus are anticipated to overcome the storage limit challenge for conventional material, promising to be the next-generation of high density spintronic devices [1]. Current-driven skyrmion motion such as rotation and translation using low current density has been realized in skyrmion lattice crystals [2]. Alarmingly, such a current-driven motion occurs at temperatures far below room temperature and suffers a narrow manipulation temperature window. This raises the crucial question whether the formation of the skyrmion lattices can be manipulated by electric-current at room temperature, while simultaneously achieving wide-temperature stability. Here, we introduce a centrosymmetric MnNiGa compound showing the individual biskyrmion magnetic nanodomains at room temperature [3]. This allowed for first time to direct observation of the change of the isolated biskyrmions into ordered lattices, which can be electrically manipulated forming 1/0 bit-like carriers needed in magnetic storage. The application of electric-current substantially reduced the threshold magnetic field to form the biskyrmions and makes biskyrmion lattice to survive even without magnetic field. This easy and efficient tuning options together with fascinating topological features such as nanometric localized spin configuration and robust biskyrmions lattices with the uniform chirality makes this material excellent candidate for technical application as information carriers in the next generation ultra-dense magnetic spintronic devices.

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Oral Tue3-01

Heavy Weyl fermion state in $CeRu_4Sn_6$

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A new type of topological state in strongly correlatted condensed matter systems, heavy Weyl fermion state, has been found in a heavy fermion material $CeRu_4Sn_6$, which has no inversion symmetry. Both two different types of Weyl points, type I and II, can be found in the quasi-particle band structure obtained by the LDA+Guztwiller calculations, which can treat the strong correlation effects among the f-electrons from Cerium atoms. The surface calculations indicate that the topologically protected Fermi arc states exist on the (010) but not on the (001) surfaces.

Symmetry and topology in topological semimetal materials

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Topological structure of electronic wavefunctions has lead us to seminal discoveries on topological insulators. The notion of topology in electronic wavefunctions is now extended to metals, leading us to a new topological phases of topological semimetals. In such topological semimetals, the band gap closes at generic points or lines, due to topological reasons. In this presentation we show our recent results on topological semimetals, such as Weyl semimetals and nodal-line semimetals.

Weyl semimetals (WS) [1-3] are semimetals with nondegenerate 3D Dirac cones in the bulk. In the presentation we show that in a transition between topological and ordinary insulators, the Weyl semimetal phase necessarily appears, for any inversion-asymmetric crystals [1,2,4]. Namely, if the gap of an inversion-asymmetric system is closed by a change of an external parameter, the system runs either into (i) a Weyl semimetal phase or (ii) a nodal-line semimetal [4]. This transition is realized for example in tellurium (Te). Tellurium has a unique lattice structure, consisting of helical chains, and therefore lacks inversion symmetry. At high pressure the band gap of Te decreases and it runs into a Weyl semimetal phase, as shown by our *ab initio* calculation [5].

We also show by *ab initio* calculations that fcc Ca (calcium) have topological nodal lines near the Fermi level when the spin-orbit interaction is neglected [6]. These nodal lines are purely topological, characterized by the π Berry phase. In Ca at high pressure, only the nodal lines lie at the Fermi level, and it is a nodal-line semimetal. This nodal line gives rise to a wavevector region with π Zak phase (Berry phase), which leads to a large amount of surface polarization charge [6].

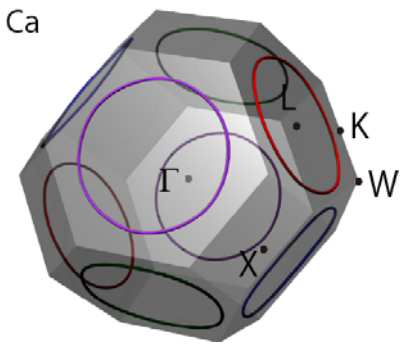

Fig.1: Nodal lines in calcium

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Oral Tue3-03

Phase Transitions and Topology in the Exciton-Polariton Condensate of the Gapped 2D Dirac Materials

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For the quantum well in an optical microcavity, the interplay of the Coulomb interaction and the electron-photon coupling can lead to the emergence of bosonic quasiparticles consisting of the exciton and the cavity photon known as polariton, which can form the Bose-Einstein condensate above a threshold density. Additional physics due to the nontrivial Berry phase comes into play when the quantum well consists of the gapped Dirac material such as the transition metal dichalcogenide (TMD) MoS2 or WTe2. Specifically, in forming excitons, the electron-photon coupling from the optical selection rule due to the Berry phase competes against, rather than cooperates with, the Coulomb interaction. We find that this competition gives rise to the spontaneous breaking of the rotational symmetry in the polariton condensate and also drives topological phase transition, both novel features in polariton condensation. We also investigate the possible detection of this competition through photoluminescence.

Quantum Magnetotransport in Topological Semimetals

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Weyl semimetals are three-dimensional topological states of matter, in a sense that they host electrons that could mimic massless relativistic particles with linear dispersion in three-dimensional momentum space, i.e., the long-sought Weyl fermions in high energy physics. It inherits many of the properties of Weyl fermions, including the violation of chiral charge conservation or chiral anomaly. Searching for the signature of the violation of chiral charge conservation in solids has inspired a growing passion on the magneto-transport in topological semimetals. One of the open questions is how the conductivity depends on magnetic fields in a semimetal phase. Several recent experiments on both Weyl and Dirac topological semimetals show unconventional behaviors in transport measurement. Here I introduce theories of magnetoconductivity of Weyl and Dirac semimetals in several different regimes, including the weak antiloclization in a weak field, negative magnetoresistance induced by chiral anomaly, a purely quantum mechanical phenomenon, and magnetoresistance in a strong field.

Superconducting proximity in three-dimensional Dirac materials: Majorana fermions from pseudo-scalar pairing

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When a conventional BCS superconductor is brought into contact with a normal metal, only singlet (scalar) superconductivity can be induced into the metal. However when it is brought to contact with a three dimensional Dirac material (3DDM), in principle 16 forms of different superconducting orders can be induced the properties of which depend on whether the Dirac material has one or a pair of Dirac valleys [1]. Fiertz decomposition of the induced superconductivity shows that in 3DDM with a single Dirac cone depending on the chemical potential, scalar, pseudo-scalar, four-vector, pseudo-four-vector and tensor valued superconducting order are possible. For Dirac materials with two valleys, four-vector, tensor and pseudo-four-vector superconducting orders are possible. Fermion doubling renders the first two of the above superconductivities into odd-frequency pairing [2]. We then examine all of the above superconducting orders with respect topological charge. We find that the pseudo-scalar superconductivity of 3DDM is able to close the mass gap of the Dirac equation itself whereby a two-dimensional sea of Majorana fermions is created [3]. This mechanism of generation of Majorana fermions does not require p-wave superconductors, nor the time-reversal symmetry breaking magnetic fields and therefore avoids complications related to presence of gapless excitation in the vortex core [4].

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Majorana zero mode with spin selective Andreev reflection inside vortex of topological superconductor

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We present a theory for Majorana zero mode with spin selective Andreev reflection inside vortex of topological superconductor, and calculate spin polarization dependence of the scanning tunneling conductance. The results are compared with the recently reported experiment by Jia et al to support the evidence of the Majorana zero mode inside vortices in $Bi_2Te_3/NbSe_2$ hetero-structure, in which topological superconductivity was previously established.

Quantum Criticality and Superconductivity in Heavy-Fermion Compounds

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There are now multiple examples of unconventional superconductivity developing as the Néel temperature of a heavy-fermion antiferromagnet is tuned by pressure toward T=0, a quantum critical point (QCP). These examples are most obvious in Ce-based heavy-fermion systems, and though there is no microscopic theory of the superconducting mechanism, qualitative arguments suggest that an attractive d-wave pair interaction is induced by quantum-critical magnetic excitations at momenta of the initial spin-density wave order.[1] There is, however, the possibility that the criticality could be of a qualitatively different nature.[2] We discuss evidence for two different types of pressure-induced quantum criticality in a single material $CeRh_{0.58}Ir_{0.42}In_5$ and the relationship of these criticalities to superconductivity. This study allows a broader perspective on quantum criticality in a family of Ce-based heavy-fermion antiferromagnets and superconductors whose ground states appear to be controlled by orbital anisotropy of their 4f wavefunctions.

*Work at Los Alamos was performed under the auspices of the US DOE, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering. In collaboration with Y. Luo and P. F. S. Rosa.

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STS studies on correlated *f*-electron systems: the fate of the Kondo lattice

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Electronic correlations give rise to a plethora of interesting phenomena and phases. For example, hybridization between 4*f* and conduction electrons in heavy fermion metals may result in the generation of low-energy scales that can induce quantum criticality and unconventional superconductivity[1]. One of the most important techniques that helped shaping our understanding of nonlocal correlations, both magnetic and superconducting, has been scanning tunneling spectroscopy (STS) with its unique ability to give local, microscopic information that directly relates to the one-particle Green's function. We combine STS with bulk measurements to obtain complementary information on different length scales.
We studied the temperature evolution of hybridization effects and Kondo lattice coherence as observed by STS, focusing on the model heavy fermion metal $YbRh_2Si_2$ and the intermediate-valence insulator SmB_6. Investigation of high-quality single crystals of $YbRh_2Si_2$ allows to study evolution of the signatures of the development of Kondo lattice coherence upon lowering the temperature[2]. We also show how Kondo coherence connects with quantum criticality[3]. These results by STS are compared to magnetotransport and thermodynamic measurements, as well as to findings on other heavy fermion materials. Low-temperature *in-situ* cleaving of SmB_6 single crystals mostly resulted in reconstructed surfaces, while non-reconstructed patches were found less frequently. The different surface terminations give rise to marked differences in the STS results[4]; in our analysis, however, we concentrate on STS of non-reconstructed areas. These spectra confirm the hybridization picture typically considered for this material[5]. At the surface, the Kondo effect is suppressed to lower temperatures as compared to the bulk material[6]. All types of surfaces, reconstructed and non-reconstructed, displayed a finite zero-bias conductance of considerable magnitude confirming the robustness of the metallic surface states.

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Hidden Order in URu_2Si_2: A spin-dependent orbital density wave phase

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We investigate a model (the under-screened Anderson lattice model [1]) that supports a phase transition which leads to a reconstruction of the Fermi-surface and breaks perioic translational symmetry and spin-rotational invariance. The transition is driven by the spin-flip terms of the Hund's rule exchange interaction. The order parameter is of a combined spin and orbital character and so that it does not have super-lattice peaks that can be observed in either x-ray or neutron scattering experiments, and thereforte may possibly desribe the hidden ordered phase of URu2Si2. We show that [2], lthough the low temperature phase of the model does not exhibit staggered magnetic moments, the suceptibility becomes anisotropic below the critical temperature. This type of symmetry breaking has previously been reported by Okazaki *et al.* [3] for URu2Si2. We show that under the application of pressure, the hidden ordered phase becomes unstable by a first-order transition to a large moment antiferromagnetic phase, as has been previously observed by Amitsuka *et al*. [4]. We show that the applicaton of a magnetic field drives the hidden ordered phase towards a quantum critical point. However, the phase boundary abruptly changes from second-order to first-order before the quantum critical point has been reached. The decrease in the magnitude of the critical temperature with applied field and the change in the order of the transition is consistent with the measurements of the specific heat anomaly by Jaime *et al*. [5].

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Kitaev interaction in hexagonal iridates and rhodates

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Heavy transition metal oxides with large spin orbit coupling and threefold coordinated effective ½ spins are discussed as promising materials to realize a particular bonding dependent anisotropic exchange called Kitaev interaction, which supports topological quantum spin liquid behavior. In this context, I will present recent results on two-and three-dimensional honeycomb iridates and rhodates.

Work in collaboration with F. Freund, A. Jesche, R. Manna, S. Manni, I. Pietsch, Yogesh Singh, S. Choi, S. Williams, R. Coldea, P. Khuntia, M. Baenitz.

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Progress in comparison of ARPES to DMFT for *d* and *f* strongly correlated electron systems

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The comparison of angle-resolved photoemission (ARPES) to dynamical mean field theory (DMFT) electronic structures is reviewed for three correlated electron systems of V_2O_3, $CeCoIn_5$ and SmB_6. The electronic structure of metallic phase V_2O_3, key to understanding its various metal-insulator transitions with temperature, doping and pressure, is revealed by ARPES [1] to have a *d*-orbital band filling that is inconsistent with a 2007 DMFT model of correlation-enhanced orbital polarization, but is thematically consistent with more recent DMFT calculations stressing full charge-self-consistency.

The Kondo lattice system $CeCoIn_5$ is shown to exhibit *itinerant f*-electron participation in the *localized-like* 3D Fermi surface topology consistent with the low energy scale description of DMFT calculations, and with a temperature-dependence that extends far above the transport coherence temperature of $T^*\sim45$K [2].

Finally, the temperature-dependent evolution of the bulk 4*f* electronic structure of mixed-valent SmB_6 revealed by ARPES and DMFT [3] identifies an important role in *f-p* hybridization assistance to the metal-insulator transition (MIT) beyond the minimal two-band models of *f-d* hybridization. The current status of the topological insulator scenario for the SmB_6 in-gap surface states is also reviewed.

Work is done in experimental collaboration with Sooyoung Jang, J. W. Allen, M.B. Maple, Jeongsoo Kang, Dae-Jeong Kim, Z. Fisk, Irene Lo Vecchio and Alessandra Lanzara, and theory collaboration with Chang-Jong Kang, B. I. Min, Jae Nyeong Kim, Bo-Gyu Jang and J. H. Shim.

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Extraordinary Coulomb Correlations of Weyl fermions in an organic conductor

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Electron correlations constitute major sources of interests in the exploration of novel electronic properties. For Weyl fermion systems consisted of massless electrons with conical dispersion, the interparticle Coulomb interaction is expected to be highly unusual since its long-range component is unscreened at the band-crossing Weyl nodes due to the vanishing density of states, affecting drastically the nature of fermions as established in quantum electrodynamics. In the present work, the site-selective NMR spectroscopy and resistivity measurements combined with model calculations find that the anisotropic Weyl fermions appearing in a quasi-two-dimensional organic conductor possess an extraordinarily strong Coulomb correlation, which was indicated by the following observations.

i) **Nonuniform Weyl-cone reshaping or velocity enhancement that developes toward the Weyl poits[1]**: our theoretical analyses based on the renormalization-group approach show that the cone reshaping is a direct consequence of the long-range part of the Coulomb interaction.
ii) **An anomalous ferrimagnetic spin polarization induced by magnetic field[1]**; this is accounted for by the short-range part of the Coulomb interaction, as revealed by a simulation based on the Hubbard model.
iii) **A thousand times enhancement of the Korringa ratio (the NMR index of spin correlations) from the values in conventional metal[2]**: our model calculations based on renormalization-group treatment reveal that it arises from the short-wavelength correlations that persist at low energy despite the drastic suppression of the long-wavelength correlations by the running Coulomb coupling.
iv) **A sudden increase of the dynamic spin susceptibility (probed by the NMR relaxation rate) at low temperatures[2]**: which is identified by model calculations within the ladder approximation as indicating spin-triplet excitonic fluctuations – precursors to mass generation associated with chiral symmetry breaking.
v) **Insulating resistivity behavior at low temperatures[3]**: this can signify the precursor of the excitonic condensation.

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Oral Wed3-01

Correlated states near electronic and structural instabilities

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Many complex materials display an interesting interplay between structural and electronic instabilities which can be studied effectively under applied pressure. This talk will present some recent examples, including (i) a structural quantum critical point and its consequences for superconductivity in the quasi-skutterudite system $(Sr/Ca)_3(Ir/Rh)_4Sn_{13}$, (ii) unconventional superconductivity in YFe_2Ge_2 and its connection with superconductivity in the high-pressure collapsed tetragonal phase of alkaline-metal iron arsenides, and (iii) strong-coupling superconductivity in the incommensurate high-pressure host-guest structure of elemental bismuth.

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Exact critical exponents for the antiferromagnetic quantum critical metal in two dimensions

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Unconventional metallic states which do not support well defined single-particle excitations can arise near quantum phase transitions as strong quantum fluctuations of incipient order parameters prevent electrons from forming coherent quasiparticles. Although antiferromagnetic phase transitions occur commonly in correlated metals, understanding the nature of the strange metal realized at the critical point in layered systems has been hampered by a lack of reliable theoretical methods that take into account strong quantum fluctuations. We present a non-perturbative solution to the low-energy theory for the antiferromagnetic quantum critical metal in two spatial dimensions. Being a strongly coupled theory, it can still be solved reliably in the low-energy limit as quantum fluctuations are organized by a new control parameter that emerges dynamically. We predict the exact critical exponents that govern the universal scaling of physical observables at low temperatures.

Parity-broken monatomic-layer superconductors

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One or two atomic layers grown on crystal surfaces are recently found to be superconducting: a monolayer of Pb [1,2,3], two atomic layers of In [1,2] and Ga [4], and a monolayer of Tl+Pb alloy [5] on Si(111) surface, a single unit layer of FeSe [6,7] film, Ca-intercalated double-layer graphene [8], and so on. Interesting points of these 'atomic-layer superconductors' may be three fold; (1) Two-dimensionality, (2) Influence of substrates, and (3) symmetry breaking.

(1) Two dimensionality (2D): According to Mermin-Wagner Theorem, 2D lattices do not have phase transitions due to large fluctuation. This means no superconductivity in monatomic layers. But in reality, even monatomic layers are not strictly 2D, but 'quasi-2D' having a finite thickness due to spread of electron wavefunction in surface-normal direction, which results in atomic-layer superconductivity. In addition, we can expect Berezinskii-Kosterlitz-Thouless (BKT) transitions in the atomic-layer superconductivity, in which unusual low-temperature phases are expected having exponentially decaying correlation with distance. We have experimentally observed the large fluctuation and BKT transition at atomic-layer superconductors [5].

(2) Influence of substrate: The superconducting transition temperatures T_C of most of the known atomic-layer superconductors are lower than those of the bulk materials. This is believed to be due to the interaction with the substrates. One exception is the single unit-layer FeSe film which shows T_C higher than 100 K while that of the bulk FeSe crystal is a few K [5,6]. One explanation for this is interface phonons which are effective for Cooper pairing. This example indicates possibility to enhance T_C by making materials as thin as monolayer thick on suitable substrates.

(3) Symmetry breaking: Since the material surfaces are in a situation of break-down of space-inversion symmetry, spin degeneracy in electronic states can be lifted (Rashba effect) [5]. Superconductivity at surfaces and monolayers are then novel because singlet- and triplet-Coopers can be mixed (parity-broken superconductivity). Actually, scanning tunneling spectra taken from the superconducting (Tl+Pb) monolayer is not reproduced by BCS theory based on *s*-wave superconductivity. This may be a breakthrough in research exploring new types of superconductivity.

In my talk I will show some experimental data of *in situ* four-point probe transport measurements and ultra-low temperature scanning tunneling microscopy/spectroscopy on some atomic-layer superconductors, and discuss the future. This work is based on collaboration with the groups of A. A. Saranin, A. V. Zotov in Russia, and Y. Hasegawa at ISSP of Univ. Tokyo.

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Emergent magnetic anisotropy in cubic $CeIn_3$

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Metals containing cerium exhibit a diverse range of fascinating phenomena including heavy fermion behavior, quantum criticality, and novel states of matter such as unconventional superconductivity. Because spin-orbit coupling and crystal field energy scales are large relative to the energy scales of the associated phenomena it is generally believed to be safe to assume that the interactions between the f-electrons are spherically symmetric in spin space. By using magnetic fields with strengths comparable to the crystal field energy scale we illustrate the breakdown of the spherical approximation in the prototypical cubic heavy fermion material $CeIn_3$, which also displays unconventional superconductivity near a quantum critical point under applied pressure. Above 40 T, the H-T phase diagram develops a surprising anisotropy. This work demonstrates that magnetic anisotropy must be included in modeling f-electron materials, when the orbital character of the 4f wavefunction changes (e.g. with pressure or composition). In addition, magnetic fields are shown to tune the effective hybridization and exchange interactions potentially leading to new exotic field tuned effects in f-based materials.

Oral Thu1-02

NMR Studies on U-based Ferromagnetic Superconductors

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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 the 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 FM ordering and superconductivity originate from U 5*f* electrons [5], resulting in the microscopic coexistence of ferromagnetism and superconductivity 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 ($H//c$) strongly suppresses both the FM Ising-type fluctuations and superconductivity in the same manner [7]. In addition, $1/T_1$ in the field along the *b* axis (H^b) becomes enhanced above $\mu_0 H^b > 5$ T, indicating that the FM fluctuations are enhanced. Interestingly, the superconducting critical field also increases with increasing fields, indicating that the superconductivity becomes robust in the same H^b region [8]. These results strongly suggest that the characteristic FM fluctuations tuned by external fields induce unique spin-triplet superconductivity in UCoGe, which is also supported by the recent Knight-shift measurements in the superconducting state [9].

We will introduce recent NMR results on single-crystal URhGe [10,11] and UGe_2 done by other groups, and discuss the similarity and difference in these superconductors.

The NMR/NQR studies on single-crystal UCoGe were done in the collaboration with T. Hattori, M. Manago, K. Karube, Y. Ihara, K. Deguchi, N. K. Sato, and T. Yamamura.

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First-principles dynamical mean field theory approach on heavy fermion system

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In *f* electron-based heavy fermion compounds, the temperature dependent behavior of the *f* electron is determined by the competition between Kondo effect and RKKY interaction. The *f* electron's magnetic moments bind to the itinerant quasiparticles to form composite heavy quasiparticle bands at low temperature to produce a large Fermi surface. When the *f* electrons are localized free moments, a small Fermi surface is induced with the absence of coherent contribution from *f* electrons. In the dynamical mean field theory approach of Ce-based heavy fermion compounds, we addressed that the Fermi surface sizes and their effective masses show continuous logarithmic scaling behavior (~ $\ln(T_0/T)$) with different characteristic temperatures.[1,2] Under the pressure or chemical doping, the temperature scale can be changed which is related to the movement of the quantum critical point.[3,4] Also, the role of crystalline electric field (CEF) to the spectral function has been investigated in $YbRh_2Si_2$ with well-defined CEF splitting. We describe the CEF multiplet Kondo resonance peaks similar to recent experimental observation [5] and suggest that the CEF effect enhances the localization of the Yb ions under pressure.[6]

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What is going on in the nematic phase of iron based superconductor?

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Recently, the nematic phase, the electronic phase with symmetry lowered down to C2 from C4 rotational symmetry while the crystal symmetry remains under C4 symmetry, became a major playground of iron-based superconductor research by virtue of its exotic nature as well as its possible connection to the superconductivity. However, the microscopic mechanism has not been made, even the driver of the nematic phase is unclear so far.

In this talk, I will present two electronic structure study results by mean of angle resolved photoemission spectroscopy that could give us a new insight on the nematic phase. One result contains a separation of orbital order and magnetic order realized in surface-electron-doped $BaFe_2As_2$. The other result presents the occupation reversed ferro-orbital order in FeSe bulk crystal where long-range magnetic order does not set in. With these two results, I will discuss the role of orbital degree of freedom on the nematic phase of iron-based superconductor.

Spectroscopic-imaging STM studies of superconductivity and nematicity in $FeSe_{1-x}S_x$

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Spontaneous breaking of lattice rotational symmetry in the electronic state, which is known as electronic nematicity, has been observed in various materials including unconventional superconductors such as cuprates and iron-based materials. In order to make clear the relationship between superconductivity and nematicity, we have performed spectroscopic-imaging STM on $FeSe_{1-x}S_x$. The parent material FeSe undergoes tetragonal-to-orthorhombic transition at 90 K, which is a manifestation of electronic nematic order. Superconductivity sets in at lower temperature of 9 K. The electronic nematic order is suppressed with increasing sulfur content x and disappears above $x \sim 0.17$, whereas superconducting transition temperature remains intact[1]. We have investigated the evolution of the band structure as a function of x by analyzing the quasiparticle interference patterns. We have found that anisotropy of the in-plane band structure diminishes with increasing x but there is little change in the band structure at $x = 0.17$. Superconducting gap is hardly affected by sulfur doping in the nematic phase but is suddenly smeared once the nematic phase diminishes. This result indicates that superconductivity and nematicity are strongly interrelated.

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Oral Thu2-03

Spin-fluctuation-driven preformed singlet pairs in the iron-pnictide, $Na_{1-x}Li_xFeAs$

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In this talk, I will present a nuclear magnetic resonance (NMR) study of the Li-doped NaFeAs single crystals. The successful incorporation of Li into the parent NaFeAs is evidenced by the progressive evolution of the ^{75}As NMR spectra as a function of doping x. Our NMR data show that the local static and dynamic properties of the system drastically change through $x_c \sim 0.03$ above which long-range spin-density-wave (SDW) order disappears and, at the same time, bulk superconductivity emerges abruptly. Strikingly, despite the absence of static moments at $x > x_c$, the spin-lattice relaxation data reveal a clear phase transition occurring at a characteristic temperature T_0 just above the superconducting transition temperature T_c, that resembles the SDW transition. The data indicate that the phase transition at T_0 accompanies the formation of singlet pairs of electrons driven by antiferromagnetic spin fluctuations, gapping the spin excitation spectrum. Upon further lowering temperature, the system enters a bulk superconducting state, strongly suggesting that the preformed electron pairs become coherent Cooper pairs at $T_c < T_0$.

Ferromagnetic Van der Waals Metal Fe_3GeTe_2: from Bulk to Atomically Thin Crystals

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Atomically-thin crystals, recently realized using van der Waals (vdW) materials, provide a versatile platform for studying the stability and tunability of the correlated electron phases in reduced dimension. Here, we present the thickness dependence of the phase transition in the layered ternary metal chalcogenides, Fe_3GeTe_2, hosting the ferromagnetic (FM) phase at T_c ~ 220 K, highest among vdW ferromagnets. In ultrathin crystals, even with a thickness of five unit cells, we observed the stable FM ground state and large anomalous Hall effect. The clear correlation between T_c and the in-plane saturation field demonstrate that the uniaxial magnetic anisotropy is essential for stabilizing the FM phase, confirming two-dimensional nature of ferromagnetism.

Oral Thu3-02

Intertwinded orders in Mott-Kitaev honeycomb iridates

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Honeycomb iridates are thought to have strongly spin-anisotropic exchange interactions that could potentially lead to an extraordinary state of matter known as the Kitaev quantum spin liquid. The realization of this state requires almost perfectly frustrated interactions between the magnetic Ir4+ ions, but small imbalances in energy make other ordered states more favorable. Indeed, the closeness in energy of these states is itself a signature of the intrinsic frustration in the system. We have found that small magnetic fields can be employed to drive the frustrated quantum magnet β-Li2IrO3 between different broken symmetry states, but without causing a true thermodynamic phase transition. This field- induced broken symmetry has all the signatures of a thermodynamic order parameter, but it is never truly formed in zero field. Rather, it is summoned when the scales of frustration are appropriately tipped, intertwined with other nearby quantum states.

Switching Chiral Solitons for Algebraic Operation of Topological Quaternary Digits

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Chirality is a ubiquitous and interesting property of asymmetry in many fields ranging from biology, chemistry to physics. Because of its topologically distinct nature, such chirality in condensed matter can be used to carry information robustly against external perturbations. For instance, nanoscale magnetic skyrmions, spatially localized chiral spin texture with particle-like properties in ferromagnets, have been investigated intensively as topological information carriers for next generation spintronic devices. However, logic operations using topological excitations such as skyrmions are only conceptually proposed. On the other hand, chiral solitons are recently discovered as the topologically protected edge states of one-dimensional Z_4 topological insulators [1,2], which can be exploited as topological information carriers in electronic system.

In this talk, I show experimentally and directly that switching between solitons with different chirality is possible by merging them with achiral solitons [3]. This chiral switching corresponds to the realization of topological addition of the Z_4 topological number or chirality. With their distinct topologically protected chirality, chiral solitons could uniquely be applied for robust multilevel information storage and logic operation by storing, carrying, and switching three differently topological bits of information. Furthermore, we are using solitons travelling in indium atoms on a silicon surface, and we imagine that this structure that could be implemented in current silicon devices, creating hybrid systems in near future.

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Oral Thu4-01

Topological vacuum bubbles of anyons

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According to the linked cluster theorem of fermionic and bosonic many-body physics, physical observables are not affected by vacuum bubbles, which represent virtual particles created from vacuum and self-annihilating without interacting with real particles. In this talk, we show that this conventional knowledge must be revised for anyons. We find that a certain class of vacuum bubbles of anyons, involving topological braiding of virtually excited anyons around real anyonic excitations, affects physical observables. We develop a theory of such topological vacuum bubbles for both of Abelian anyons [1] and non-Abelian anyons [2]. These topological vacuum bubbles can be detected in a fractional quantum Hall system accessible in current experiments, providing a tool for observation of elusive fractional Abelian/non-Abelian exchange statistics.

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Towards Topological and Unconventional Superconductivity

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There is great interest in finding new states of matter at the interface between topological and superconducting materials. Exfoliation and van-der-waals heterostructures have opened an entirely new route to this pursuit, with most efforts focused on conventional s-wave superconductors. In this talk I will discuss a related method our group has developed enabling a proximity effect between high Tc cuprate superconductors and various Dirac materials. In addition to providing evidence for the proximity effect, I will discuss new excitations we have observed at the interface between topological materials and high Tc cuprates as well as Fe chalcogenides.

Oral Fri1-01

Topologies and Emergent Phenomena of Domain walls in Quantum Materials

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Engineering of domains and domain boundaries is quintessential for technological exploitation of numerous functional materials. However, it has only recently realized that the configuration of these domains/domain boundaries can have non-trivial topology. We will discuss a new topological classification scheme of domain/domain boundary configurations with Ising-type or two-dimensional order parameters: Zm×Zn domains (m directional variants and n translational antiphases) and Zl vortices (where l number of domains and that of domain boundaries merge). This classification, with the concept of topological protection and topological charge conservation, has been applied to a wide range of materials such as improper ferroelectric $R(Mn,Fe)O_3$, antipolar $In(Mn,Ga)O_3$, hybrid improper ferroelectric $(Ca,Sr)_3Ti_2O_7$, chiral (and ferromagnetic) $Fe_{1/3}TaS_2$, and magnetic (and superconducting) Sr_2VO_3FeAs. We will also discuss the emergent physical properties of domain boundaries, distinct from those of domains. The presented topological consideration provides a basis in understanding the formation, kinetics, manipulation and property optimization of domains/domain boundaries in complex materials.

The anomalous de Haas-van Alphen effect and Excitons in a topological Kondo insulator

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The de Haas-van Alphen effect, describing oscillations of the magnetization as a function of magnetic field, is commonly assumed to be a definite sign for the presence of a Fermi surface (FS) in a metal. Here we show that, in contrast to this canonical situation, there can be quantum oscillations even for insulators of certain types [1,2]. We draw connections to recent experiments on the topological Kondo insulator (TKI) candidate SmB$_6$ [1]. In addition, we show that TKIs are susceptible to the formation of bound electron-hole pairs [3]. These excitons can account for long-standing thermodynamic and recent transport anomalies in SmB$_6$ which is crucial for the identification of bulk topological signatures.

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Oral Fri1-03

Symmetry enforced semimetals and symmetry enriched topologically ordered state in nonsymmorphic crystals

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Among 230 space groups, there are 157 nonsymmorphic space group having glide reflection or screw rotation symmetries. We discuss their unique distinction compared to other symmorphic groups. Based on the extended "Hastings-Oshikawa-Lieb-Schutz-Mattis" theorem, we argue that topologically trivial insulators are forbidden at certain integer fillings of particles and study their exotic low energy properties. In addition, we discuss how such nonsymmorphic symmetries lead to symmetry enforced semimetals and study their interesting phase transitions.

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Novel quantum states of matter and fractionalized excitations emergent in Kitaev materials

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Mott insulators with spin-orbit entangled $j=1/2$ Kramers doublets provide a novel platform for unconventional types of magnetism, dubbed Kitaev interactions. Local magnetic moments interacting via these bond-directional interactions on a honeycomb and a triangular lattice give rise to the formation of quantum spin liquids and non-trivial spin textures. In this talk, I will discuss our group's endeavor to observe the predicted exotic states of matter in Kitaev magnets.

In the search of a Kitaev honeycomb lattice, the 4*d* compound α-$RuCl_3$ (Ru^{3+};$4d^5$) is regarded as a prime candidate, being in proximity to a Kitaev spin liquid. Our specific heat and inelastic neutron scattering measurements establish a spin fractionalization to two kinds of Majorana fermions. This is corroborated by a two-stage release of magnetic entropy by (R/2)ln2 as well as by quasielastic excitations at low energies around the Brillouin zone center and a hour-glass-like magnetic continuum at high energies. A related question is the existence of quantum spin liquids in the three-dimensional analogue of the honeycomb iridates, β-and γ-Li2IrO_3. Using polarization-resolved Raman spectroscopy, we find that the temperature dependence of the Raman spectral weight is dominated by the thermal damping of fermionic excitations, similar to α-$RuCl_3$. Finally, the intriguing interplay of geometric and exchange frustration is investigated in the hexagonal perovskite $Ba_3IrTi_3O_9$, which is made of a mixture of edge- and corner-sharing triangles. The *T*-linear and –squared dependence of the magnetic specific heat and a persistent spin dynamics of the muon spin relaxation are indicative of spinon excitations that are a hallmark signature of a spin liquid state.

Oral Fri2-02

3D Kitaev Spin Liquids

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The Kitaev honeycomb model has become one of the archetypal examples of topological phases of matter. Being one of the few highly frustrated spin models that are exactly solvable, it has shaped our understanding of quantum spin liquid phases in general.
In this talk, we discuss the rich physics arising in generalizations of the Kitaev model to three-dimensional lattice structures. These models have low-energy degrees of freedom that are Majorana fermions, and that in general form metallic states [4]. Depending on the underlying lattice structure, these can be (almost) conventional metals with a Majorana Fermi surface [1] or Dirac semi-metals, where the gapless modes form Fermi lines or even Weyl nodes [2]. The resulting quantum spin liquids differ not only in their experimental signatures (for instance the specific heat), but also in their response to perturbations, such as an external magnetic field or additional interactions [3].
This work was done in collaboration with Kevin O'Brien[1], Achim Rosch[1], and Simon Trebst[1].

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Doping effects on 2D triangular multiferroic $Y(Mn,Al,Ga)O_3$

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Hexagonal multiferroic $RMnO_3$ is one of the most extensively studied systems [1]. In addition to the multiferroic behavior, it also hosts a two-dimensional (2D) triangular lattice of Mn moments, which itself is interesting from a magnetic point of view as a 2D triangular lattice with antiferromagnetic interaction has strong frustrations. As one way of studying the 2D nature of magnetism, several attempts have been made to dope at the Mn site with a limited success up to a nominal value of 10% [2]. Generally doping perturbs the magnetic ground state, in this case a so-called 120° noncollinear antiferromagnet. Moreover, non-magnetic impurities can also induce so-called impurity-induced spin texture, which can add further interesting feature [3-5]. In this study, we report a successful growth of doped single crystals with as much as doping of 25% of Al and Ga using a floating zone furnace. Using these single crystals, we have carried out extensive studies of physical properties as well as neutron diffraction measurements. We will discuss the experimental data with respect to expected impurity effects of ferroelectricity and magnetism.

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Poster I #02

Magnon phonon hybridization in multiferroic RMnO3

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Magneto-electric coupling (ME coupling) in multifferoic materials is an actively studied subject. In many multiferroic compounds, spin lattice coupling is believed to play important role in ME coupling. However, detailed experimental probe of such coupling Hamiltonian is rare. Here we study magnon phonon coupling in multiferroic RMnO3 by using inelastic neutron and x-ray scattering technique. The observed spectra showed clear evidence of magneto-elastic excitation and electromagnon, which are reproduced by a spin lattice coupling Hamiltonian. Furthermore, the magneto-elastic excitation shows unusual damping even at low temperatures, much below TN. We will discuss the origin of such damping and implication of our findings on the ME coupling in RMnO3..

Properties of highly frustrated antiferromagnets: Cu$RE_2Ge_2O_8$ (RE=Pr,Nd,Sm~Tm)

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Cu$RE_2Ge_2O_8$ has a monoclinic crystalline structure (space group $I\,1\,m\,1$) with rare earth polyhedrons [1] which form honeycomb like tunnel structure along its a-axis. Even though its crystal structure is not likely to allow geometrically frustrated exchange interaction, our physical property measurements show some clues of frustration. We identify crystal structure of Cu$RE_2Ge_2O_8$ system [2] using single crystal and powder X-ray diffraction methods and provide magnetization and specific heat capacity measurement data which correspond to properties of highly frustrated antiferromagnets.

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Poster I #04

Low energy spin dynamics of rare-earth orthoferrites $YFeO_3$ and $LaFeO_3$

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$YFeO_3$ and $LaFeO_3$ are members of the rare-earth orthoferrites ($RFeO_3$) family with *Pbnm* space group. With the strong superexchange interaction between Fe^{3+} ions, both compounds exhibit the room temperature antiferromagnetic order ($T_N > 600$ K) with a slight spin canting. Here we report low-energy magnetic excitation of $YFeO_3$ and $LaFeO_3$ using inelastic neutron scattering measurements, showing evidence of magnon mode splitting and a spin anisotropy gap at the zone center. Spin wave calculations with the spin Hamiltonian including both Dzyaloshinsky-Moriya interaction and single-ion anisotropy accounts for the observed features well. Our results offer insight into the underlying physics of other $RFeO_3$ with magnetic rare-earth ions or related Fe^{3+}-based multiferroic perovskites such as $BiFeO_3$.

Transport study on antiferromagnetic van der Waals $MnPS_3$ using conductive atomic force microscopy

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After the successful isolation of graphene, the field of van der Waals (vdW) materials and the list of vdW systems have grown recently at an alarming rate.[1-3] Among them, we are very interested and welcome the recent entry of new magnetic vdW materials: Transition metal phosphorus tri-chalcogenide ($TMPX_3$). Successful exfoliation has been recently demonstrated down to monolayer of these materials.[4-6] So far all the initial characterization has been made by using Raman and AFM, and there has been no report of the transport characteristics of few-layer $TMPX_3$ which is an essential step for future device applications. Thus, we have investigated the tunneling transport of mono- and few-layers of $MnPS_3$ by using conductive atomic force microscopy.[7] Due to the band alignment of indium tin oxide/$MnPS_3$/Pt-Ir tip junction, the key features of both Schottky junction and Fowler-Nordheim tunneling (FNT) were observed for all the samples with varying thickness. Using the FNT model and assuming the effective electron mass (0.5 me) of $MnPS_3$, we estimate the tunneling barrier height to be 1.31 eV and the dielectric breakdown strength as 5.41 MV/cm. We expect that these values of tunneling barrier and dielectric breakdown strength would be helpful for many applications such as field effect transistor and magnetic tunnel junction.

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Poster I #06

Strong thermal hysteresis of Verwey transition in Fe_3O_4 Nanoparticles

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Fe_3O_4 which is well-known for strongly correlated electron system has the metal-insulator transition [1] and its transition temperature decreases in nm-sized case [2] which is related to intrinsic size effect. Additionally, we found a strong thermal hysteresis in nanoparticles, whereas 7 μm bulk sample has a weak hysteresis about 1 K. Hysteresis has size dependence that its width increases up to 10 K as increasing size until 120 nm and then decreases down to 1 K. We could examine that this feature comes from the single domain structure determined by the ratio between remanent magnetization (M_r) and saturated magnetization (M_s). Theoretical calculation for possible critical size which can have a single domain [3] is similar with our results. Therefore, we could conclude that our nanoparticles have almost single domain and it makes hysteretic metal-insulator transition. Moreover, from RIXS spectra, we could observed the low energy excitation and it was gradually suppressed as reducing sizes which can describes intrinsic size effect of nanoparticles.

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Breakdown of dimerized valence bonds in $Li_2Ru_{1-x}Mn_xO_3$

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RVB(Resonating Valence bond) is a state proposed by P. W. Anderson. By this bizarre phenomenon, spins of two ions that participate in bond are predicted to be entangled [1].

Li_2RuO_3 which has 2D honeycomb layer made with ruthenium layer is a candidate of a medium of the phenomenon. One third of pair of bond in the hexagonal layer are shorter than other ruthenium bonds, also they have a long range ordering called herring bone structure. This structure has phase transition above 550 K [2][3], the dimerized bonds are melted and become a liquid of valence bond state up to 650 K [4]. For melting the bonds, I substituted Ru ion with Mn ion. As a result, the dimerized valence bonds are broken and the phase transition was vanished above 1/8 substitution.

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Poster I #08

Spin glass behavior in ultrathin magnetic van der Waals materials

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Transition metal phosphorous tri-chalcogenide, TMPS3(TM=Mn,Fe,Co,Ni) can be used for the realization of 2D magnetic properties because thickness can be reduced easily by so-called scotch tape method[1]. In recent researches, TMPS3 can be cleaved to monolayers[2] and also magnetic properties of 2D FePS3 were studied[3]. TMPS3 shows the different spin Hamiltonian depending on transition metals; 2D XY Hamiltonian(NiPS3), 2D Heisenberg (MnPS3), 2D Ising(FePS3)[4]. However, if two transition metals are mixed, it is ambiguous that which Hamiltonian this sample follows or that thickness dependence. $Mn_{0.5}Fe_{0.5}PS_3$ has been known that spin glass behaviors are shown below freezing temperature. So thickness study of spin glass is not also interesting but able to be a chance to understand the spin glasses more exactly.

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Spin dynamics in the spin chain compound Sr_3CuPtO_6

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Antiferromagnetic spin chain systems have attracted considerable attention since the discovery of fractional spinon excitations in spin-half chain systems and Haldane gap phases in spin-one chain systems. It has been reported from bulk susceptibility and heat capacity measurements that the magnetic Cu^{2+} ions in Sr_3CuPtO_6 exhibit S=1/2 Heisenberg spin chain behavior with a substantial amount of AFM interchain coupling. We report the magnetic excitation spectrum as measured by inelastic neutron scattering for a polycrystalline sample of Sr_3CuPtO_6. Modeling with linear spin wave theory accounts for the major features of the spinwave spectra, including a nondispersive intense magnon band at 8meV. The magnetic excitations broaden considerably as temperature is increased, persisting up to above 100K and displaying a broad transition as previously seen in the susceptibility data. No spin gap is observed in the dispersive spin excitations at low momentum transfer, which is consistent with Haldane physics in an ideal uniform S=1/2 spin-chain system.

Poster I #10

Evidence of electron-phonon interaction in single crystal of (Ru^{3+}/Ru^{4+}) mixed-valence $Na_{2.7}Ru_4O_9$ and $NaRu_2O_4$

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We report a comprehensive investigation of the structural, electric transport, magnetic, and thermodynamic properties of $Na_{2.7}Ru_4O_9$ and $NaRu_2O_4$ single crystals. The compounds are structurally different; $Na_{2.7}Ru_4O_9$ crystalize in monoclinic (C 2/m) structure while $NaRu_2O_4$ crystalize in orthorhombic (P 2_1/ma) structure. We observed a first-order phase transition in the electrical resistivity at T_c = 335 K and T_c = 530 K for $Na_{2.7}Ru_4O_9$ and $NaRu_2O_4$, respectively. The electrical resistivity data are then theoretically analysed within the framework of the classical electron–phonon model of resistivity, *i.e.* the Bloch–Grüneisen–Mott model. Detailed analysis of the electrical resistivity of both Ru-based metallic systems $Na_{2.7}Ru_4O_9$ and $NaRu_2O_4$ suggests that the charge carrier density is strongly influenced by electron–phonon scattering and additionally inter-band electron scattering for $Na_{2.7}Ru_4O_9$. The characteristic Debye temperature (θ_ρ) is found to be 140 and 499 K for $Na_{2.7}Ru_4O_9$ and $NaRu_2O_4$, respectively. Magnetic susceptibility $\chi(T) = M/H$ curve shows diamagnetic behaviour for both the compounds and no magnetically ordered state was observed down to 1.9 K. The evidence for metal-like electronic contribution in the low-temperature heat capacity was also observed for both the compounds. The electronic contribution to the specific heat (γ) for $Na_{2.7}Ru_4O_9$ and $NaRu_2O_4$ was determined to be 26.91 and 3.93 mJ/mol K^2, respectively. The higher value of γ for $Na_{2.7}Ru_4O_9$ is much larger than the free electron value of 1 mJ/mol K^2 Ru, indicates that $Na_{2.7}Ru_4O_9$ belongs to the class of strongly correlated electron system.

Spin Precession Pumped by Pulsed Terahertz Magnetic Field in $YMn_xFe_{1-x}O_3$

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We studied spin precession in canted antiferromagnetic $YMn_xFe_{1-x}O_3$ (x=0-0.45) by utilizing the pulsed magnetic field in terahertz light. Both the quasi-ferromagnetic resonance (qFMR) and quasi-antiferromagnetic resonance (qAFMR) modes were observed in YFeO3 (x=0). With increasing Mn doping, the qAFMR gradually disappeared, whereas the qFMR did not. We tracked the qFMR as a function of temperature. Spin reorientation transitions and new infrared-active absorption modes were also observed.

Poster I #12

Metallic Terahertz Metamaterials Research

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We performed finite-difference time-domain (FDTD) simulations of both intaglio metamaterials of NbN films and copper-meshed films on terahertz-transparent substrates in the spectral range from 0.1 to 3 THz and measured their optical conductivity by using terahertz time-domain spectroscopy. NbN-film metamaterials with oblique-DSRR (double split ring resonator) patterned structures exhibited open and closed resonance modes emerging from the low frequency region. Copper-meshed films with a honeycomb patterned structure exhibited smaller scattering rate than the basal copper film. By focusing on the average of current density and electric field within the unit cell of the meta-structure, the FDTD simulation demonstrates that the metamaterial film could be considered as a new effective medium in the wavelength region with the wavelength longer than the structural dimension.

Effect of strong spin-orbit coupling of anion p orbitals on superexchange interaction

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Recent studies on the strong spin-orbit coupling (SOC) reveals many new physics like Jeff = ½ mott state [1], Kitaev Hamiltonian [2], and Rashba splitting [3]. The efforts on the SOC driven new physics are still going on. The chalcogenide systems opens a new way with strong SOC on anion sites; 500 meV for Te 5p, and 220 meV for Se 4p [4]. We have pay attention on the effect of SOC on the superexchange interaction in 90 degree geometry, which favor ferromagnetic spin-spin interaction. Interestingly, some superexchange hopping paths can be open or closed depending on the spin direction and their effects do not cancel each other's. These on-off behavior results a magnetic anisotropy described by anisotropic Heisenberg spin-spin interaction. We have done 4 site full multiplet cluster calculation and found that the plane contain transition metals and anions become easy plane, and the energy difference are order of 0.1 meV. We have applied this anisotropy in layered chromium chalcogenides Cr2Ge2Te6 and CrI3, which realize 90 degree superexchange interaction. They are ferromagnetic correlated insulator with Tc = 78 K for Cr2Ge2Te6 and Tc = 61 K for CrI3 and saturated moments are almost 3 μB/Cr [5]. The magnetic easy axes are c direction in both systems, but conventional single site anisotropy and shape anisotropy prefer ab plane as magnetic easy plane. We propose that this discrepancy can be explained by the anisotropy driven by SOC.

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Poster I #14

Magnetic properties of epitaxially grown high quality LaCrO3 films by pulsed laser deposition

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We succeeded in epitaxial growth of $LaCrO_3$ (LCO) thin films on TiO_2 terminated $SrTiO_3$ (001) substrate by pulsed laser deposition method with a sintered stoichiometric LCO target. Atomically flat surface and its high crystallinity were confirmed by atomic force microscope and x-ray diffractometer, respectively. Stoichiometry of high crystalline film was measured by X-ray absorption spectroscopy, showing only Cr^{3+} valence feature and eventually indicating that our sample has a single phase. In bulk system, LCO exhibits the G-type antiferromagnetic ordering below the Neel temperature (T_N) of 288K. The Cr $L_{2,3}$, edge X-ray magnetic linear dichroism (MLD) and its temperature dependence were used to investigate magnetic properties of the epitaxial LCO film and its transition temperature. The results show existence of antiferromagnetic ordering in the film with the T_N of around 240K. The configuration interaction model calculations including the full atomic multiplets and crystal field splitting match well to the obtained MLD line shape and suggest the antiferromagnetic spin axis.

High-Resolution Soft X-ray RIXS Using Active Gratings and Energy Compensation

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We will present a new RIXS beamline, which is based on energy compensation principle and built for the Taiwan Photon Source. A unique technique is applied for the high-efficiency, high-resolution beamline and spectrometer of inelastic soft X-ray scattering (RIXS). This new technique is based on the energy compensation principle of grating dispersion. The design of the monochromator–spectrometer system greatly enhances the data acquisition efficiency at least by one order of magnitude. The setup comprises two bendable gratings to effectively diminish the defocus, coma and high order aberrations. A proto-type RIXS beamline of this design has been constructed at the Taiwan Light Source, showing total energy resolutions of 65 meV and 130 meV at 710 eV and 930 eV, respectively [1,2]. This test beamline has yielded successful RIXS experiments of cuprate superconductors [3]. A new RIXS beamline based on this design will be constructed at the Taiwan Photon Source. To eliminate the grating surface intrinsic slope error and heat-load deformation, a novel 25-points grating bender system is designed. A CCD detector with a sub-pixel spatial resolution through a centroid algorithm will be used. Our simulations shows that the expected energy resolving power is better than 60,000 from 500 eV to 1000 eV, with an efficiency one order of magnitude better than that of a conventional design.

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Poster I #16

Jahn-Teller distortion driven magnetic polarons in magnetite

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The first known magnetic mineral, magnetite (Fe_3O_4), has unusual properties which have fascinated mankind for centuries; it undergoes the Verwey transition at T_V ~120 K with an abrupt change in structure and electrical conductivity. The mechanism of the Verwey transition however remains contentious. Here we use resonant inelastic X-ray scattering (RIXS) over a wide temperature range across the Verwey transition to identify and separate out the magnetic excitations derived from nominal Fe^{2+} and Fe^{3+} states. Comparison of the RIXS results with crystal-field multiplet calculations shows that the spin-orbital *dd* excitons of the Fe^{2+} sites arise from a tetragonal Jahn-Teller active polaronic distortion of the $Fe^{2+}O_6$ octahedra. These low-energy excitations, which get weakened for temperatures above 350 K but persist at least up to 550 K, are distinct from optical excitations and best explained as magnetic polarons.

Electronic structure of $Ce_3Co_4Sn_{13}$ using hard X-ray photoelectron spectroscopy & x-ray absorption spectroscopy

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The compound $Ce_3Co_4Sn_{13}$ is a heavy fermion system which exhibits a charge density wave (CDW) phase transition at ~155 K [1, 2]. In the present study, we used hard X-ray photoelectron spectroscopy (HAXPES) and x-ray absorption spectroscopy (XAS) to investigate the electronic structure of $Ce_3Co_4Sn_{13}$. HAXPES measurements are carried out below and above the CDW transition using an incident photon energy of hν ~6.480 keV. Core levels and valence band spectra of $Ce_3Co_4Sn_{13}$ have been measured at 20 K and 170 K temperature. A small finite change (~90-110 meV) in the binding energy is observed across the CDW transition for the Sn 3p and Co 2p core level spectra, while Ce 3d core level shows negligible change. This observation is consistent with a recent x-ray fluorescence study at the Ce L (≡ 2p)-edge and Co K (≡ 1s)-edge [2]. Further, valence band spectra show a feature at ~1.5 eV binding energy, which is attributed to Co 3d partial density of states. In the CDW phase, the valence band spectra show a clear Fermi edge, which is consistent with the metallic behavior observed by electrical resistivity in the CDW phase[1]. Similar to HAXPES results, the XAS spectra for Co L (≡ 2p)-edge also shows an energy shift of (~90 meV), while Ce M (≡ 3d)-edge shows negligible change. The present HAXPES & XAS study suggests very weak charge-disproportionation in $Ce_3Co_4Sn_{13}$ across the CDW transition.

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Poster I #18

Raman Study on Photostrictive Perovskite $SrIrO_3$ Thin Films

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Photostrictive effect is a light-matter interaction which generates a reversible mechanical deformation in a material by illumination of light, which is also called "photostriction". Materials which possess photostrictive property can serve as energy conversion system, wireless remote control, photo sensor and so on, offering gifted potential towards novel photonic devices. However, the light-induced lattice changes in most of photostrictive materials are very small so that there are no practical applications hitherto. In this study, we investigated the visible-light-induced deformation of perovskite SrIrO3 (SIO), taking advantages of its strong spin-orbit coupling, sizable crystal field and high absorption across the visible spectrum at room temperature. By using Raman spectroscopy, the Raman mode assignments were made by group theory and the phonon behaviors of the SIO thin film under various incident laser intensities were analyzed. The phonon deformation potential of SIO was calculated by lattice mismatch induced Raman shift, and the photon-induced strain is then obtained. We found that SIO shows significant photostriction compared to conventional semiconductors, polymers and perovskite oxides under the same experiment configuration. The strong photostrictive effect of SIO at room temperature paves a promising route towards new applications and multifunctionalities of photon-driven devices.

Heteroepitaxy of Fe_3O_4/Muscovite: A New Perspective for Flexible Spintronics

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Spintronics has captured a lot of attention since it was proposed. It has been triggering numerous research groups to make their efforts on pursuing spin-related electronic devices. Recently, flexible and wearable devices are in a high demand due to their outstanding potential in practical applications. In order to introduce spintronics into the realm of flexible devices, we demonstrate that it is feasible to grow epitaxial Fe_3O_4 film, a promising candidate for realizing spintronic devices based on the tunneling magnetoresistance, on flexible muscovite. In this study, the heteroepitaxy of Fe_3O_4/muscovite is characterized by x-ray diffraction, high-resolution transmission electron microscopy, and Raman spectroscopy. The chemical composition and magnetic feature are investigated by a combination of x-ray photoelectron spectroscopy and x-ray magnetic circular dichroism. The electrical and magnetic properties are examined to show the preservation of the primitive properties of Fe_3O_4. Furthermore, various bending tests are performed to show the tunability of functionalities and to confirm that the heterostructures retain the physical properties under repeated cycles. These results illustrate that the Fe_3O_4/muscovite heterostructure can be a potential candidate for the applications in flexible spintronics.
Keywords: Heteroepitaxy, Spintronics, Magnetite, Muscovite, Flexible electronics

Poster I #20

Van der Waals Epitaxy of Flexible and Transparent VO_2 Film on Muscovite

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A strong demand on electronic devices with new functionalities triggers researchers to explore new materials or architecture design that silicon-based electronics cannot reach. A great attention has been paid to Vanadium dioxide (VO_2). The crystal structure of VO_2 can be transformed between the rutile and monoclinic phases accompanied by a first-order metal-insulator transition (MIT). This transition is fully reversible and the T_c of the MIT is very close to room temperature. More importantly, the structure transition of VO_2 happens at ultrafast timescale and can be triggered by multiple approaches, making it very attractive to practical applications. Recently, flexible electronics represents a fast-developing field and has a strong impact to our daily life. However, to fabricate high-quality VO_2 on flexible substrates remains a grand challenge. Traditionally, high-quality VO_2 thin films can be deposited on the rigid substrates. In this study, the growth of VO_2 film directly on a transparent and flexible muscovite via van der Waals epitaxy is established. The unique metal-insulator transition of VO_2 is further revealed with a change in electrical resistance over 10^3 and a more than 50% variation of optical transmittance. Furthermore, due to the nature of muscovite, the VO_2/muscovite heterostructure possesses superior flexibility and optical transparence. The approach developed in this study paves an intriguing way to fabricate functional VO_2 film for the applications in flexible electronics.

High Mobility Transparent Heteroepitaxy (Ba, La)SnO_3/Muscovite for Flexible Optoelectronics

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Transparent conducting oxides (TCOs) play an important role in modern optoeletronic applications such as solar cells, flexible displays and sensor devices. As there is an increasing demand in next generation devices with high performance, improving the mobility is an essential issue for developing transparent logic devices. In this study, we propose the Lanthanum-doped barium stannate (Ba, La)SnO_3 – a new TCO with high electron mobility in perovskite structure – which captured significant attention in the last decade. Recent studies have focused on the advanced synthesis as well as the intriguing properties of (Ba, La)SnO_3. In this work, we introduce pulsed laser deposition process to synthesize heteroepitaxial (Ba, La)SnO_3 thin film on transparent flexible muscovite. This combination not only elegantly exhibits excellent electrical properties but also enhances optical and flexible characteristics. Our study offers a pathway to fabricate flexible transparent high-power functional devices for optoelectronic applications.

Keywords: high mobility, Lanthanum doped barium stannate, perovskite, transparent conducting oxides, muscovite

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Poster I #22

Creating Flexoelectrity via Composition gradient

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Complex oxides present versatile properties, such as ferroelectricity, superconducting, and colossal magnetoresistance, making the complex oxides is widely studied. To improve or manipulate the properties, complex oxides are designed and well grown into different structures, from thin film of single material to hetero-structure combined at least two materials. As the advancement of growth technique, the accuracy can be controlled into a unit cell via the assistance of reflection high energy electron diffraction (RHEED). Hence, a new type of hetero-structure is proposed as shown in Fig. 1. Utilizing the ability to control the growth in the atomic scale, a non-uniformity with composition gradient along the out-of-plane (OOP) direction is created. The model system is constituted by $SrTiO_3$ (STO) and $LaAlO_3$ (LAO). Under this circumstance of OOP composition gradient, a strain gradient is accompanied. Polarity discontinuities between STO and LAO are also expected compared to the bi-layer system[1]. Through the coupling among the charge, orbital and lattice, a spontaneous polarization is created. As the spontaneous polarization is induced and manipulated by strain gradient, we name it "flexoelectricity". This study is expected as a model system of periodic non-uniformity to design the artificial charge/spin density wave.

[1] Nature 427, 423-426 (2004).

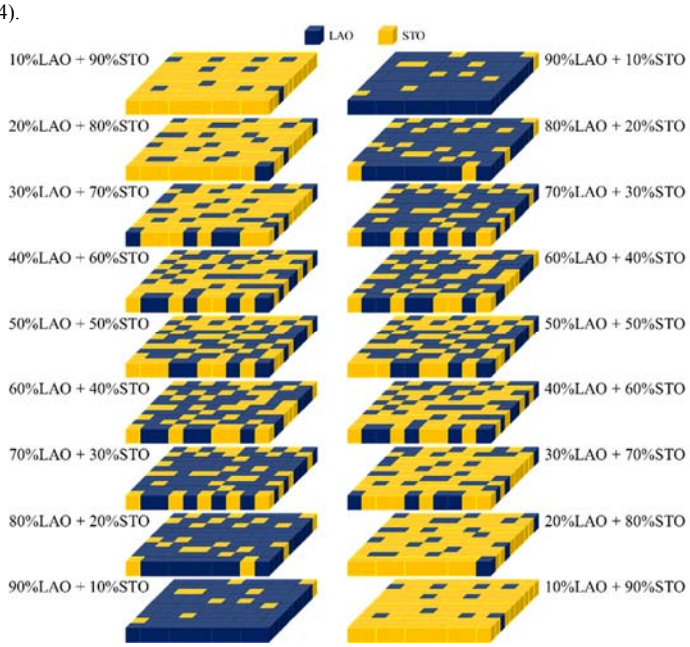

Figure 1. The schematic of LAO-STO composite system. The thickness of each layer is a unit cell.

Search for complex orbital order in magnetite Fe_3O_4 by magnetic-field-direction dependent XAS and XMCD measurements

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The nature of the Verwey transition of magnetite Fe_3O_4 at ~120K showing a large conductivity jump has been controversial for many decades. Recently, two theoretical models for the low-temperature phase were proposed. One is the charge-(real-)orbital order [1] model and the other is the charge-complex-orbital order (COO) [2] model.

In order to examine the validity of these models, we have performed angle-dependent x-ray magnetic circular dichroism (XMCD) measurement above and below the Verwey transition temperature T_V on a thin film sample grown on a stepped MgO substrate (the twin of the Verwey order was suppressed by the epitaxial strain from the step edges) .

As shown in Fig. 1, we obtained the magnetic field direction dependence of the orbital magnetic moment. We also found changes in the spectral line shape depending on the magnetic field direction and temperature (XMCD spectra of three different temperatures and magnetic field directions are shown in Fig. 2 (a) and (b), respectively for example). These behavers are well explained by the COO model.

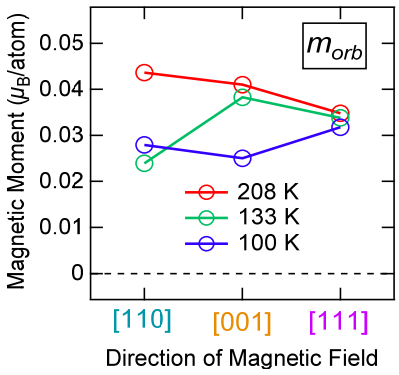

Fig.1 Magnetic field direction dependence of the orbital magnetic moment deduced from XMCD.

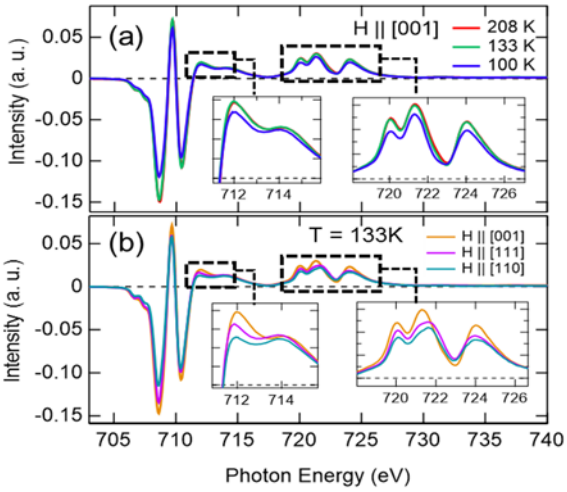

Fig. 2 XMCD spectra obtained under different conditions. (a) Spectra at three different temperatures under the magnetic field of 1T along the [001] direction. (b) Spectra for three different magnetic field directions under 133 K.

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Poster I #24

High-Pressure Synthesis of a Third-Family Perovskite Bismuthate

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Perovskite bismuthates have been widely known to be a parent compound of high-T_c superconductors, namely, $Ba(Pb,Bi)O_3$ (T_c = 13 K)[1] and $(Ba,K)BiO_3$ (T_c = 30 K)[2]. Since the first-family compounds were found, subsequent studies have continued and led to the discovery of a second-family compound $(Sr,K)BiO_3$ with $T_c \sim 12$ K[3]. A central question is to understand the role of structural distortions driven by A-site ion[4], and to control the distortions further by designing a new material. Here, we report the first synthesis of a third-family of perovskite bismuthates, $CaBiO_3$, using a high-pressure technique. A stoichiometric mixture of CaO_2, Bi, and Bi_2O_3 powders was reacted at 850 °C, 6 GPa, for 1 hour using a cubic anvil apparatus (TRY Engineering, 500-ton press). Structural refinement using power XRD revealed a perovskite $CaBiO_3$ phase, with the smallest and lowest-symmetry lattice structure among the bismuthate families. These results suggest that $CaBiO_3$ could be applied to elucidating the relation between lattice distortions and superconductivity in bismuthates.

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Structure analysis of LaNiO 3 /LaAlO 3 interface by surface X-ray diffraction

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The perovskite oxide LaNiO 3 (LNO) shows a metallic behavior over the whole temperature range. When we make LNO ultrathin films thinner than 2 monolayers on the analogous material LaAlO 3 (LAO), the films exhibit an insulating behavior . Several scenarios have been proposed for this insulating ground states such as dimensional-crossover [1] and local field given by the surface termination [2]. However, interfacial structure of LNO/LAO as a function of the thickness has not been clarified. In this study, we performed surface x-ray diffraction experiments on LNO/LAO interfaces (1~5 monolayer) at BL-4C and 3A of the Photon Factory, KEK to clarify interfacial structure of LNO/LAO and investigate the origin of its insulating ground state. Unit cell volume of metallic (4~5 unit cell thick) LNO was found to be larger than that of insulating (2~3 unit cell thick) ones. Internal electric field estimated by the cation displacements shows little difference among the samples measured.

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Poster I #26

The pressure effect on magnetoelectricity in Cr_2O_3

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In recent years, the linear magnetoelectric (ME) effect in which electric polarization (magnetization) is linearly induced by applied magnetic field (electric field) attracts large attention because this effect is expected to be used for fabricating new-type devices based on the electric-field control of magnetism. However, there are few materials that display such an effect at room temperature and the magnitude of the effect is too small to use for practical use. Chromia, Cr2O3, is the most classical compound which represents the linear ME effect below the Néel temperature *T*N≈307 K. In this study, we investigated the effect of hydrostatic pressure on magnetic and ME properties in single crystals of Cr2O3. To elucidate *T*N under high pressure, we measured dielectric constant at various pressures by using a clamp cell and a diamond anvil cell. Since *T*N corresponds to a ME phase transition temperature, the dielectric constant exhibits a divergent anomaly at *T*N in the pressure of a magnetic field through the ME coupling. Thus, dielectric measurements can be a sensitive probe to determine *T*N in Cr2O3. Our result clearly shows the enhancement of *T*N in Cr2O3 by applying hydrostatic pressure. More detail of the result will be presented.

Novel relaxation behaviors in the orbital-ordered vanadates

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Relaxation phenomena have been observed in various materials, for example, CMR manganites [1], where the spin degree of freedom plays an important role. We found that $Ba_{1-x}Sr_xV_{13}O_{18}$ and $Ba_{1-x}Sr_xV_{10}O_{15}$ exhibit a time-dependent resistivity and susceptibility, which is caused by the novel relaxation phenomena dominated by the orbital/charge degrees of freedom in the V ions.

$Ba_{1-x}Sr_xV_{13}O_{18}$ and $Ba_{1-x}Sr_xV_{10}O_{15}$, in which the average of valence of the V ions is +2.62 and +2.8 respectively, have orbital/charge degrees of freedom in the V ions. $Ba_{1-x}Sr_xV_{13}O_{18}$ exhibits three different phases with temperatures [2,3]: The high-temperature (HT) phase is characterized by three V tetramers and a lone V ion in the unit cell. In the intermediate temperature (IT) phase, the unit cell is doubled, indicating a charge ordering with a localized *d* electron in the lone V ion. In the low temperature (LT) phase, the V tetramers are decomposed and changed into V trimers. $Ba_{1-x}Sr_xV_{10}O_{15}$ also exhibits three different phases [4,5]: the HT phase with no ordering, the IT phase with the tripling of the unit cell, and the LT phase with the V trimerization.

We measured the time dependence of the electrical resistivity and the magnetic susceptibility for the single crystals of these compounds. We found that with a rapid cooling rate (>50K/min), the IT phase survives down to the lowest temperature as a metastable phase for both compounds. We observed a time dependence of the resistivity and the magnetic susceptibility when the temperature is slightly increased after such a rapid cooling, indicating a relaxation from the IT phase to the LT phase in both compounds. Furthermore, we found that $Ba_{1-x}Sr_xV_{10}O_{15}$ exhibits a percolative relaxation, whereas $Ba_{1-x}Sr_xV_{13}O_{18}$ exhibits a relaxation with an exponential decay.

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Poster II #01

Al doping effect on helical magnet CrAs under pressure

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Pressure-induced superconductivity was recently discovered in the helical magnet CrAs. When subjected to the external pressure, the antiferromagnetic (AFM) transition temperature decreases to zero temperature and a superconducting phase is induced near the AFM state [1, 2]. The close proximity of the SC phase to a T = 0 K AFM transition indicates a possible interplay between the two broken symmetries. Here we report the Al substitution effects for As, where the AFM ordering temperature T_N increases to 275 K from 265 K of the undoped CrAs. T_N gradually decreases under pressure up to 4 kbar and is completely suppressed at about 4.7 kbar, which is lower than 7 kbar for the undoped compound. Superconducting state emerges when T_N is completely suppressed and T_c maximum occurs near 10 kbar. Strong enhancement of the electrical resistivity (ρ) is centered around 4.7 kbar, the critical pressure where T_N is extrapolated to zero Kelvin. The clear separation between the projected AFM QCP and the optimal pressure of T_c maximum suggests that the attractive interaction required for producing SC Cooper pairs may not arise from the AF quantum fluctuations in the Al-doped CrAs.

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Anisotropic upper critical field in the pressure-induced superconductivity for the single crystal of CrAs

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We investigate anisotropy of upper critical field (γ_{Hc2}) for CrAs single crystals under pressure. The CrAs shows an antiferromagnetic (AFM) phase transition at T_N ~ 264 K at ambient pressure, where the long-range AFM order and magnetostriction simultaneously occur. When the crystals are subjected to the pressure, the T_N is rapidly suppressed with increasing pressure and disappears at the critical pressure (P_c ~ 7 kbar) where the bulk superconductivity is induced. With further increasing pressure, the superconducting phase shows a dome shape centered around 10 kbar. The upper critical field ($\mu_0 H_{c2}$) for the CrAs under pressure shows anisotropic behavior for magnetic field applied parallel ($H//a$) and perpendicular ($H \perp$ a) to the crystalline a-axis. The $\gamma_{Hc2}(T)$ for the CrAs shows a similar behavior with multiband superconductors, such as MgB_2, Fe-based superconductors suggesting that the pressure-induced superconductivity in the CrAs is associated with a multiband nature.

PACS numbers: 74.25.F-, 74.25.Op, 74.62.Fj, 74.70.Xa
keywords: CrAs, upper critical field, pressure, anisotropy

Poster II #03

Band Dependent Pseudogap Opening in Iron Pnictide Sr_2VO_3FeAs

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In cuprate unconventional superconductor, a gap, so called pseudogap, remains even above the superconducting transition temperature (Tc). Because of its unique property, the pseudogap has been studied to clarify the origin of it. However, debates on the origin of the pseudogap are still on-going. Recent discovery of iron-based superconductors can allow a new chance to approach the longstanding issue on the unconventional superconductors. In practice, the similar phase diagram of iron-based superconductors to that of cuprates suggest that the pseudogap can exist in iron-based superconductor1.

In this study, we have performed angle-resolved photoemission spectroscopy measurement on Sr_2VO_3FeAs, which has moderately high Tc of 37 K[2] and multiple bands at Fermi level[3]. As a result of the measurement, we observed different gap behavior in each band of Sr_2VO_3FeAs that the pseudogap opening in the hole band, while no gap exists above Tc in the electron band. This band dependent dichotomous pseudogap opening may suggest that the observed pseudogap is driven by orbital instability, not by preformed Cooper pairs in this system. Even though the pseudogap study is necessary in other iron-based superconductor systems to understand the dichotomous pseudogap nature more clearly, this result can provide a new insight on the pesudogap issue.

Multiple Fulde-Ferrel-Larkin-Ovchinnikov states in FeSe

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Superconductivity is conventionally described as a spin-singlet state with zero net momentum arising from pairing of electrons with opposite spins and momentums. When spin population is imbalanced, however, an exotic spin-singlet superconducting state, called the Fulde-Ferrel-Larkin-Ovchinnikov (FFLO) state, may occur with nonzero net momentum and spatially modulated order parameter. While relatively well-established is the nature of the FFLO state in single-band superconductors, whose order parameter modulation is determined by a single length scale, more complex evolution of the FFLO phases in multiband superconductors has remained as a challenging issue. In multiband superconductors, competition between the FFLO phases with different modulation length scales, set by multiple Fermi surfaces, leads to rich phase transitions under magnetic elds, which is yet to be observed in real systems. Here, we report the multiple field-induced anomalies in FeSe below its upper critical field showing a clear low-temperature upturn, which is consistent with proposed characteristics of the multiband FFLO state. Our observations implies that FeSe, atypical iron-based superconductor, represents a unique model system for the multiband FFLO states.

Poster II #05

Emergent electronic phases in a hetero-structured iron-based superconductor

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In heterostructures, subtle balance of competing interactions between the layers can generate new exotic phases that would otherwise not be stabilized in either layer. Here, we report that one such example is the natural heterostructure of a Mott-insulating vanadium oxide and a high-Tc superconducting iron pnictide. Using high-quality single crystals of Sr_2VO_3FeAs we provide evidence that an emergent electronic phase is developed at $T_0 \sim 155$ K in the FeAs layer of Sr_2VO_3FeAs without accompanying either static magnetism or crystal symmetry change. Significant interlayer coupling between itinerant iron electrons and localized vanadium spins suppresses the otherwise strong antiferromagnetic and C_2 nematic instabilities and induces the unusual spin-gapped and C_4 orbital-ordered ground state. This emergent electronic phase in Sr_2VO_3FeAs is drastically distinct from the phase transitions found in other iron pnictides or vanadium oxides, highlighting the importance of the interlayer coupling in this system.

Evidence of nodeless multigap superconductivity in 2H-Pd_xTaSe_2 from London penetration depth and thermal transport

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2*H*-$TaSe_2$ is a renowned charge density wave (CDW) system which shows an incommensurate charge density wave (ICDW) at ≈ 122 K followed by a commensurate charge density wave (CCDW) at ≈ 90 K and superconductivity at T_c ~ 0.14 K. Recently, it has been observed that upon systematic intercalation of Pd ions into 2*H*-$TaSe_2$, the CCDW order is destabilized more rapidly than ICDW to indicate a hidden quantum phase transition point at x ~ 0.09 - 0.10. Furthermore, T_c shows a dramatic enhancement up to 3.3 K at x = 0.08, ~24 times of T_c in 2*H*-$TaSe_2$[1]. In this work, we measured the temperature dependence of in-plane London penetration depth (λ_{ab}) and thermal conductivity (κ_{ab}) of a 2*H*-Pd_xTaSe_2 single crystal with T_c ~ 3.13 K. In zero-field, the temperature dependence of λ_{ab} exhibits a power-law AT^n with n = 2.66 and there is no residual linear term in κ_{ab}/T at $T \rightarrow 0$. Moreover, magnetic field dependence of the normalized residual linear term ($\kappa_0(H)/T$)/(κ_N/T)) exhibits similar behavior observed in multigap superconductor like $NbSe_2$[2]. These results strongly indicate the presence of multiple nodeless superconducting gaps in 2*H*-Pd_xTaSe_2.

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Poster II #07

Non-equilibrium lattice vibrations of As ions in spin-density-wave state of $BaFe_2As_2$

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We have investigated coherent phonon oscillations of $BaFe_2As_2$ by NIR pump - NIR probe spectroscopy. On optical excitation with the spin-density-wave (SDW) order, an A_{1g} coherent phonon mode of As vibrations shows two distinct oscillation frequencies depending on probe light polarizations along the *in-plane* orthorhombic axes. It is noticeable that such a photo-induced anomaly does not appear without the order and the frequency difference of the A_{1g} mode is far from thermal lattice evolution. We suggest that although all the As ions have the same symmetry in the equilibrium state, there should be two different types of As ions in the non-equilibrium SDW state.

Hidden non-Fermi liquid properties of $BaFe_{2-x}Ni_xAs_2$ pnictides

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We studied Ni-doped Ba-122 single crystals at two different doping levels using an optical spectroscopic technique. The underdoped sample shows a magnetic phase transition around 80 K. We analyze the data with a Drude-Lorentz model with two Drude components ($D1$ and $D2$). It is known that the narrow $D1$ component originates from electron carriers in the electron-pockets and the broad $D2$ mode is from hole carriers in the hole pockets. While the plasma frequencies of both Drude components and the static scattering rate of the broad $D2$ component show negligible temperature dependencies, the static scattering rate of the $D1$ mode shows strong temperature dependence for the both samples. We observed a hidden quasilinear temperature dependence in the scattering rate of the $D1$ mode above and below the magnetic transition temperature while in the optimally doped sample the scattering rate shows a more quadratic temperature dependence. The hidden non-Fermi liquid behavior in the underdoped sample seems to be related to the magnetic phase of the material.

Poster II #09

Hydrostatic Pressure Effects on the Superconductivity of $Ca_{0.9}La_{0.1}FeAs_2$ Single Crystal

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Recently, La-doped $CaFeAs_2$ has been found to exhibit a high superconducting transition temperature ($T_c \sim 36$ K), with a superconducting volume ratio up to 66% [1]. The La-doped $CaFeAs_2$ has a conductive intermediate layer of As-As between the FeAs superconducting layers. In this work, we have grown the La-doped $CaFeAs_2$ single crystal with an improved flux method. The $Ca_{0.9}La_{0.1}FeAs_2$ single crystal grown by this method exhibits a $T_c \sim 46$ K and a large volume fraction ~ 70%. We also investigated the hydrostatic pressure dependence of resistivity in $Ca_{0.9}La_{0.1}FeAs_2$ up to 8.5GPa with the combination of a hybrid piston cell and a cubic anvil press. The pressure dependence of T_c reveals a dome shaped behavior with a maximum $T_c \sim 51.4$ K at 1.6GPa. At this pressure, T-dependence of resistivity shows a linear behavior for $T > T_c$ possibly due to the non-Fermi liquid state or multiband effect.

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Interplay of charge density wave and multiband superconductivity in 2*H*-Pd_xTaSe_2

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2*H*-$TaSe_2$ has been one of the unique transition metal dichalcogenides exhibiting several phase transitions due to a delicate balance among competing electronic ground states. An unusual metallic state at high-T is sequentially followed by an incommensurate charge density wave (ICDW) state at ≈ 122 K and a commensurate charge density wave (CCDW) state at ≈ 90 K, and superconductivity at T_c ≈ 0.14 K. Upon systematic intercalation of Pd ions into $TaSe_2$, we find that CCDW order is destabilized more rapidly than ICDW to indicate a hidden quantum phase transition point at x ≈ 0.09-0.10. Moreover, T_c shows a dramatic enhancement up to 3.3 K at x = 0.08, ≈24 times of T_c in 2*H*-$TaSe_2$, in proportional to the density of states $N(E_F)$. Investigations of upper critical fields H_{c2} in single crystals reveal evidences of multiband superconductivity as temperature-dependent anisotropy factor $\gamma_H = H_{c2}^{ab}/H_{c2}^{c}$, quasi-linear increase of $H_{c2}^{c}(T)$, and an upward, positive-curvature in $H_{c2}^{ab}(T)$ near T_c. Furthermore, analysis of temperature-dependent electronic specific heat corroborates the presence of multiple superconducting gaps. Based on above findings and electronic phase diagram vs x, we propose that the increase of $N(E_F)$ and effective electron-phonon coupling in the vicinity of CDW quantum phase transition should be a key to the large enhancement of T_c in Pd_xTaSe_2.

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Poster II #11

Magneto-transport properties in All-in-All-out magnetic ordered epitaxial $Sm_2Ir_2O_7$ and $Nd_2Ir_2O_7$ film

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Observation of quantum critical point by pressure evolution of critical current density in $CeRhIn_5$

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The quantum critical point (QCP) in the heavy fermion superconductor $CeRhIn_5$ system is hidden by pressure-induced superconductivity which makes it difficult to observe the QCP clearly. Therefore, the investigation of superconducting state related to the quantum criticality is important. In this study, we consider critical current density (J_c) to investigate the QCP inside superconducting state in the $CeRhIn_5$ system: $CeRhIn_5$ and $CeRhSn_{0.22}In_{4.78}$. Pressure evolution of J_c is not dominated by flux pinning property, but is mainly associated with the pressure evolution of superconducting coupling strength, since the pinning sites, mainly defects, are not changed by applied pressure. The hidden QCP, $P_c \sim 2.3$ GPa for $CeRhIn_5$ and $P_c \sim 1.3$ GPa for $CeRhSn_{0.22}In_{4.78}$, by the superconducting dome is clearly veiled by the $J_c(P,T)$, and the largest J_c is detected at the pressure P_c. In addition, the sudden enhancement of the J_c for both $CeRhIn_5$ and $CeRhSn_{0.22}In_{4.78}$ is developed at P_c* where the antiferromagnetic (AFM) long-range order is totally suppressed and bulk superconductivity is induced. Above the P_c*, interestingly, the magnetoresistance (MR) of $CeRhIn_5$ below $T < T_c$ is increased up to certain magnetic fields and then decreased, whereas this anomalous MR behavior is negligible in the $CeRhSn_{0.22}In_{4.78}$, suggesting that the strong AFM spin fluctuations is crucial source to induce a large T_c. This phenomenological approach for the QCP provides a new guidance to find a correlation between quantum criticality and superconductivity.

Poster II #13

Pinned Quantum Critical Point in the Hg doped $CeRhIn_5$

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$CeRhIn_5$ is a prototypical antiferromagnet where the AFM ordering temperature (T_N = 3.7 K) is suppressed with pressure to reveal an AFM quantum critical point (QCP) at the optimal pressure of 2.3 GPa, where T_c is the highest [1, 2]. A study on electrical resistivity of the 4.4% Sn-doped $CeRhIn_5$ under pressure showed that T_N was suppressed from 3.7 K to 2 K and the AFM QCP is accordingly shifted to a lower pressure of 1.3 GPa [3]. In this presentation, we report electrical resistivity of the 0.45% and 1% Hg-doped $CeRhIn_5$, a hole doping case, where T_N is suppressed to 3.4 and 2.8 K for 0.45 and 1% Hg doping, respectively. In contrast to the Sn doped compound, the AFM QCPs of both Hg doped $CeRhIn_5$ are pinned at 2.3 GPa and the optimal pressure with T_c maximum is revealed at the same pressure of 2.3 GPa. The pinned QCP in the Hg doped $CeRhIn_5$ indicates that the hole doping locally changes the electronic states surrounding the dopant, while the electron doping (or Sn doping) globally changes the electronic structure of Rh115 [4]. Even though the electron and hole doping effects are asymmetric, it is universal that the AFM QCP coincides with the optimal pressure where T_c is maximum, underpinning that AFM fluctuations from the QCP is the glue to form unconventional superconductivity in $CeRhIn_5$.

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Pressure-induced Superconducting State in $MoTe_2$

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We report pressure-induced superconductivity in a single crystal of the transition-metal dichalcogenide 1T'-$MoTe_{2-x}$. At atmospheric pressure, this material goes through a structural phase transition near 210 K but pressure induces superconductivity at 0.47 K and 0.4 GPa. With increasing pressure, the monoclinic-to-orthorhombic transition temperature (T^*) decreases and electrical resistivity measurements do not show any anomaly associated with it above 1.2 GPa, where T^* and T_c become equal. Meissner effects observed by AC magnetic susceptibility measurements underline the bulk nature of the pressure induced SC state. At 1.4 GPa, where T_c is 3.2 K, differential conductance measurements reveal the Andreev reflection, which can be explained by a single SC gap with 0.48 meV. The anisotropy in H_{c2} for field applied parallel and perpendicular to the *c*-axis at 2.5 GPa is 0.5 and almost independent of temperature. These results show that the pressure-induced SC state is a weakly coupled superconductor with the gap to T_c ratio of 3.63, which competes againstthe T_d Weyl semimetalic phase, but is stable in the 1T' monoclinic phase.

Poster II #15

Strain dependence of superconducting $BaPb_{1-x}Bi_xO_3$ thin film

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The high-T_C superconductor $BaPb_{1-x}Bi_xO_3$(BPBO, T_C=13K), which is an hole-doped state of $BaBiO_3$ (BBO), has some intriguing properties itself. In spite of BBO is an insulating material, an insulator to metal-superconductor transition is occurred with changing the doping rate *x*[1]. Furthermore, in BPBO, orthorhombic and tetragonal phases coexist over a full range of the doping rate *x* and the mechanism which leads superconducting BPBO is still ambiguous. Therefore, strain engineering of BPBO with heteroepitaxy is expected to reveal its ambiguity.

In previous research, the applicable buffer templates for BPBO was developed [2]. In this research, we prepared BPBO thin films on various buffer templates by using pulsed laser deposition technique. We characterized BPBO thin films by using X-ray diffraction(XRD) and atomic force microscopy(AFM). Subsequently, we obtained high quality BPBO thin films. We carried out transport properties of BPBO thin films with different buffer templates, respectively. As a result, we have confirmed that strain could change T_C of BPBO thin films.

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Suppression of T_c and magnetic impurity effects in the single crystals of Li($Fe_{1-x}Mn_x$)As

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Substitution of transition metal ions on the Fe-site of the Fe-based superconductors is one of the most fascinating research topic since the superconductivity arises via the substitution while most of the pristine compounds have a spin-density-wave ground state. For LiFeAs, which exhibits only a superconducting transition with T_c of ~ 18 K at the ambient condition, it is reported that the chemical substitution accompanying the introduction of additional electrons, such as Co and Ni doping, suppresses the superconductivity. Mn substitution, on the other hand, which introduces local magnetic moments instead of additional hole carriers in other compounds, has not been reported in LiFeAs, even it is expected to be a good candidate for the study of the magnetic impurity effects on the superconductivity of the Fe-based family. In this presentation, the phase diagram of Li($Fe_{1-x}Mn_x$)As single crystals is presented. The self-flux method is employed to grow high quality single crystals of Li($Fe_{1-x}Mn_x$)As. In electrical resistivity and magnetic susceptibility, T_c decreases monotonically with the increase of x. In addition, the magnetization of the crystals shows clear Curie-Weiss-like temperature dependence, which is not observed in Li($Fe_{1-x}Co_x$)As. It seems to indicate that the Mn dopants is acting as the magnetic impurities in the system. The suppression of T_c is much faster than one in not only Li($Fe_{1-x}Co_x$)As but also Li($Fe_{1-x}Cu_x$)As while both Co and Cu contents in the series are non-magnetic impurities. The contrast of the T_c suppression rate in Li($Fe_{1-x}Mn_x$)As and Li($Fe_{1-x}Cu_x$)As is consistent to the theoretical prediction of the magnetic and non-magnetic impurity effect on T_c while the calculation was based on the $s\pm$-wave gap symmetry

Poster II #17

Synthesis and characterization of the Ce-doped $LaIn_3$

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$CeIn_3$ belongs to the family of heavy fermion systems, where the Kondo exchange interactions between the 4f electrons of Ce^{3+} ions and itinerant electrons are important to understand the physical properties. It is a prototypical antiferromagnet with T_N =10.2 K, which becomes superconducting near a critical pressure where TN is suppressed to zero Kelvin. In order to probe the effects of magnetic impurities in the normal metal, we have substitute Ce for La. . In this presentation, we will discuss the physical properties of the Ce-doped $LaIn_3$ from the powder X-ray diffraction, magnetic susceptibility and electrical resistivity.

Ultrafast Terahertz Dynamics of $Ba_{0.6}K_{0.4}BiO_3$ Superconducting Thin Films

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We investigated potassium (K)-doped $BaBiO_3$ (BKBO) superconducting thin films via ultrafast terahertz (THz) experiments. For this study, we prepared optimally-doped BKBO ($Ba_{0.6}K_{0.4}BiO_3$) samples of which have different superconducting-transition temperatures T_c depending on their individual disorder levels. With low-disordered BKBO films, the THz spectra below T_c reflect the superfluid condensate and quasiparticle dynamics, both of which are in fairly consistent with a well-known THz response of BCS-type superconductors with high purity (which is well-described by a Mattis-Bardeen theory). In contrast, the highly-disordered BKBO film shows totally distinguished spectral features prominently as a resonance-like absorption at around the absorption threshold 2Δ (corresponding to superconducting gap energy in the clean limit) in the superconducting state. The unusual low-energy (THz) electrodynamics probably originates from the emergence of a new collective mode associated with Higgs-like bosons.

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Poster II #19

Development of low temperature and high magnetic field Powder X-ray diffraction facility for field-driven structural phase transition studies

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The current progress of materials science regarding multifunctional materials (MFM) has put forward the challenges to understand the microscopic origin of their properties [1,2]. Most of such MFMs have magneto-elastic correlations. To investigate the underlying mechanism, it is therefore essential to investigate the structural properties in the presence of magnetic field. Such facilities are available at synchrotron sources. However, very few such setup on Lab. sources are available worldwide [3, 4] but none in India. Keeping this in view, low temperature and high magnetic field (LTHM) powder x-ray diffraction (XRD), a unique state-of-art facility have been developed at UGC DAE CSR Indore, India [5]. The setup has 18 kW rotating anode Cu-Kα x-ray vertical line source and works in a symmetric θ-2θ parallel beam geometry. Equipped with 8T split-pair Nb-Ti superconducting magnet, comprising two wide 65° x-ray windows. 8T superconducting magnet is mounted on a non-magnetic type heavy-duty goniometer equipped with all necessary motions along with data collection accessories. Parabolic multilayer mirror is used to create parallel incident x-ray and scattered beam is detected using NaI detector with 0.1° acceptance solar collimator. The wide-angle scattering data can be collected in a range of 2°–115° of 2θ with a resolution of ~0.1°. The functioning of the goniometer and the artifacts arising possibly due to the e□ect of stray magnetic field on the goniometer motions, on the x-ray source, and on the detector have been characterized by collecting powder XRD data of a National Institute of Standards and Technology certified standard reference material LaB_6 (SRM-660b) and Si powder in zero-field and in-field conditions. Occurrence of field induced structural-phase transitions has been demonstrated on various samples like $Pr_{0.5}Sr_{0.5}MnO_3$, $Nd_{0.49}Sr_{0.51}MnO_{3-\delta}$ and $La_{0.175}Pr_{0.45}Ca_{0.375}MnO_3$ by collecting data in zero field cool and field cool conditions [6].

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Electronic structures of Ce-based Kondo insulators

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Topological Kondo insulators draw lots of recent attention, and so research on Kondo insulators is actively revived. SmB6 is a typical example. Among Ce-based systems, CeNiSn and CeRhSb have also been investigated as promising candidates of Kondo insulators, but it is controversial whether they are Kondo insulators or semimetals. Recent magnetothermoelectric measurement on CeNiSn suggested that CeNiSn is a nodal metal arising from anisotropic hybridization [1]. Specific heat and thermal conductivity measurements, however, indicate that CeNiSn has an anisotropic pseudo-gap [2]. To explore the Kondo nature in CeNiSn, we have investigated the electronic structures of CeNiSn, CeRhSb, and CeRhAs that is an isostructural material with CeNiSn, utilizing the density functional theory and the dynamical mean field theory. We have also examined the topological properties of those systems.

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Poster II #21

Ultrafast study of topological insulator Bi_2Te_3 single crystal

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We conducted optical pump-probe (OPP) spectroscopy on topological insulator Bi_2Te_3 single crystals over the temperatures ranging from 20 K to 250 K. We observed a dramatic change in the reflectivity in which the fast and slow background relaxations superimposed by coherent oscillations appear. The background relaxations might be due to the ultrafast dynamics of photoexcited charge carriers (including Dirac fermions and bulk free-carriers) while the coherent oscillations originate from the Raman-active phonons (A1g at 1.9 THz, E1g at 3.2 THz, A2g at 4.1 THz). Their tempeature- and fluence-dependent evolutions shown in our data must be crucial for unveiling a mysterious interaction mechanism between Dirac fermions and phonons.

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Unconventional topological phase transition in two-dimensional systems with space-time inversion symmetry

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We study a topological phase transition between a normal insulator and a quantum spin Hall insulator in two-dimensional (2D) systems with time-reversal and two-fold rotation symmetries. Contrary to the case of ordinary time-reversal invariant systems where a direct transition between two insulators is generally predicted, we find that the topological phase transition in systems with an additional two-fold rotation symmetry is mediated by an emergent stable two-dimensional Weyl semimetal phase between two insulators. Here the central role is played by the so-called space-time inversion symmetry, the combination of time-reversal and two-fold rotation symmetries, which guarantees the quantization of the Berry phase around a 2D Weyl point even in the presence of strong spin-orbit coupling. Pair-creation/pair-annihilation of Weyl points accompanying partner exchange between different pairs induces a jump of a 2D Z_{2} topological invariant leading to a topological phase transition. According to our theory, the topological phase transition in HgTe/CdTe quantum well structure is mediated by a stable 2D Weyl semimetal phase since the quantum well, lacking inversion symmetry intrinsically, has two-fold rotation about the growth direction. Namely, the HgTe/CdTe quantum well can show 2D Weyl semimetallic behavior within a small but finite interval in the thickness of HgTe layers between a normal insulator and a quantum spin Hall insulator. We also propose that few-layer black phosphorus under perpendicular electric field is another candidate system to observe the unconventional topological phase transition mechanism accompanied by emerging 2D Weyl semimetal phase protected by space-time inversion symmetry.

Poster II #23

Classification of gap closing process through band inversion in layer groups

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We classify gap closing process due to band inversion mediated by one external parameter in two-dimensional system with time reversal symmetry for the 80 layer groups. We find that although direct transition between insulators is predicted in the general point in the Brillouin zone even in the absence of inversion symmetry, stable semimetallic state may arise (even forced) in the presence of certain symmetries. These symmetries can be put into three classes. In the first class, a combination of time reversal symmetry and a twofold rotation about the z axis (normal to the plane) always protect Weyl points in the Brillouin zone. In the second class, a mirror symmetry with axis normal to the plane may protect a line node. In the third class, the presence of a twofold rotation or a mirror symmetry with in-plane axis may protect Weyl points along the high symmetry line in the Brillouin zone. In the second and the third class, the stability of the semimetallic phase depends on the eigenvalue spectrum of the energy bands. To clarify how gap closes, we also found the effective Hamiltonian near the critical point. The behavior of these Hamiltonians can be put into three classes. For all three classes, quadratically dispersing bands approach each other as we tune the external parameter. In the first class, the bands disperse linearly away from the gap closing point just as the bands touch, and then the gap opens. In the second class, the bands disperse linearly in one direction and quadratically in the orthogonal direction. As we further tune the external parameter, a pair of Weyl points is generated in the quadratically dispersing direction. In the Third class, the bands disperse quadratically just as the bands touch, and then a line node is formed.

Measurement of size dependent magnetoelectric coupling in Fe_3O_4 nanoparticles

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Magnetite (Fe_3O_4) is one of the well-known magnetoelectric (ME) materials wherein the ME coupling is observed at below ~10 K. However, the understanding of ME coupling in nano-sized Fe_3O_4 particles is still missing. We herein report the systematic studies on size dependence of the ME coupling in Fe_3O_4 nanoparticles embedded in insulating Stycast. We have successfully synthesized uniform sized Fe_3O_4 nanoparticles with sizes ranging from 3 nm to 15 nm. An intrinsic ME coupling in Fe_3O_4 nanoparticles is demonstrated by ME susceptibility (MES) measurement, showing the maximum MES of ~0.6 ps/m at 5 K for 15 nm. The ME signal is strongly size-dependent, decreases with decreasing particle size and completely disappears for nanoparticles smaller than 5 nm. Moreover, the critical temperatures at which MES becomes zero, increase from 9.8 K in bulk to 19.7 K in 7 nm nanoparticles. The critical temperatures in MES were further confirmed by the temperature anomalies in the magnetization.

Poster II #25

Pressure-induced insulator-metal transition in $Ca_2Ru_{0.92}Fe_{0.08}O_4$ investigated by infrared microspectroscopy

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We investigated pressure-induced insulator-metal transition in $Ca_2Ru_{0.92}Fe_{0.08}O_4$ by using infrared microspectroscopy. As the pressure is increased up to above 0.9 GPa, we observed a large increment of the reflectivity in the entire mid-infrared range. Accompanied by such a clear signature of the insulator-metal transition, we found an evidence of the structural transition from the frequency shift of the Ru-O stretch phonon mode. When we compared these pressure-dependent changes with the corresponding temperature-dependent results, we found that the pressure-induced metallic state has a higher reflectivity as well as the higher phonon frequency. Indeed, it turns out that the pressure-induced metallic state of $Ca_2Ru_{0.92}Fe_{0.08}O_4$ looks very similar with the metallic state of Sr-substituted Ca_2RuO_4 not only in the reflectivity level but also in the phonon frequency. This suggests that the electronic properties are closely related to the structural degree of freedom, and the pressure can be a useful parameter to induce the transitions from the Mott-insulator to the metal and further to the superconductor.

Role of Correlation Effect on O_2 dimer bond length and Metal-Insulator Transition of FeO_2

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Iron oxide is a key compound to understand the state of the deep Earth. It has been believed that previously known oxides such as FeO and Fe_2O_3 will be dominant at the mantle conditions. However, the recent observation of FeO_2 shed another light to the composition of the deep lower
mantle (DLM) and thus understanding of the physical properties of FeO_2 will be critical to model DLM [1]. Here, we report the electronic structure and structural properties of FeO_2 by using density functional theory (DFT) and dynamic mean field theory (DMFT). The crystal structure of FeO_2 is composed of Fe^{2+} and O_2^{2-} dimers, where the Fe ions are surrounded by the octahedral O atoms. We found that FeO_2 shows metal-insulator transition (MIT) under high pressure. The MIT is not a Mott type but a band insulator type which is driven by the O_2 dimer bond length change. However, the correlation effect of Fe 3*d* orbitals should be considered to correctly describe O_2 dimer bond length of FeO_2 and the MIT.

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Poster II #27

Ultrafast study on metal-insulator transition in 5*d* pyrochlore $Cd_2Os_2O_7$

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Metal-insulator transition (MIT) of 5*d* pyrochlore $Cd_2Os_2O_7$ is occurred with all-in-all-out (AIAO) antiferromagnetic ordering. Recent studies show that the MIT of $Cd_2Os_2O_7$ is not Slater type but Lifshitz type transition [1, 2] and suggest that antiferromagnetic metallic state exists below antiferromagnetic ordering temperature T_N = 227 K [1]. However, mechanism of MIT is not clear.

In order to explain mechanism of MIT, we investigated the metal-insulator transition (MIT) in $Cd_2Os_2O_7$ 5d pyrochlore by using optical pump-probe spectroscopy. We observed critical slowing down at magnetic ordering temperature T_N = 227 K and competition between two kinds of relaxation components below T_N. Further investigation by using optical-pump THz-probe spectroscopy is also planned for detailed study.

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Transparent *p*-CuI/*n*-BaSnO3-δ Wide Bandgap Heterojunction Diodes

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We fabricated transparent *p*-CuI/*n*-BaSnO3-δ diodes in visible spectral range with high mobility (~65 cm2V-1s-1) *n*-type semiconductor material Ba0.96La0.04SnO3 on SrTiO3 (001)
substrate. A thermally evaporated γ-CuI film exhibits preferred (111)-orientation. γ-CuI film on glass shows smooth surface root-mean square (rms) roughness (Rrms ~ 1.3 nm). A transmittance of γ-CuI is over the 80 % at visible light with wide optical bandgap (*Eg* ~ 3.09 eV). The electrical parameters from Hall effect are *p* =1.2 x 1019 cm-3, *ρ* = 11.46 x 10-2 Ωcm and *μ*h = 4.4 cm2V-1s-1 for hole concentration, electrical resistivity, and mobility, respectively. The hetero structure consists of *p*+-CuI and pulsed laser deposited *n*-BSO/BLSO on STO (001). The *p*-CuI/*n*-BaSnO3-δ heterojunction diode well rectified the current with on/off ratio about 7 x 105 at ±2 V and ideality factor (*η* ~ 1.59).

Poster II #29

Angle resolved Photoemission Spectroscopy Studies on the Surface States of $SrTiO_3$ and $KTaO_3$

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We have performed angle resolved photoemission spectroscopy studies on the bare surfaces of lightly electron doped $SrTiO_3$ (STO) and $KTaO_3$ (KTO) single crystals. Our results on the cleaved surface of STO reveals new subband structure for out-of-plane dxz/yz orbitals. Our temperature dependent data shows a significant change in the observed bands toward Fermi level. In addition, we have investigated the chiral OAM textures on STO and KTO surfaces using circular dichroism ARPES technique to discuss the origin of surface band splitting.[1,2]

Berry phase crossover in a Nodal Line Semimetal SrAs3

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Dirac electronic state have gathered interests by their unconventional electronic states characterized by intrinsic chirality of (psuedo) spins. Recently, we found that SrAs3 is a strong candidate of nodal-line semimetal confirmed by band structure calculations. We observed angular-dependent Shubnikov-de Haas (SdH) oscillations of a high-quality SrAs3 single crystal. The berry phase factor extract from landau fan diagram shows strong angle dependence. We discuss how these observations related to evidence for SrAs3 as the nodal-line semimetal.

Poster II #31

Compact localized states and flatband generators in one dimension

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Flat bands (FB) are strictly dispersionless bands in the Bloch spectrum of a periodic lattice Hamiltonian, recently observed in a variety of photonic and dissipative condensate networks. FB Hamiltonians are finetuned networks, still lacking a comprehensive generating principle. We in- troduce a FB generator based on local network properties. We classify FB networks through the properties of compact localized states (CLS) which are exact FB eigenstates and occupy U unit cells. We obtain the complete two-parameter FB family of two-band d = 1 networks with nearest unit cell interaction and U = 2. We discover a novel high symmetry sawtooth chain with identical hoppings in a transverse dc field, easily accessible in experiments. Our results pave the way towards a complete description of FBs in networks with more bands and in higher dimensions.

Doping and temperature dependence of the electronic structure of $(Sr_{1-x}La_x)_2IrO_4$

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We investigated the electronic response of $(Sr_{1-x}La_x)_2IrO_4$ by using optical spectroscopy. We observed a filling-controlled insulator-to-metal transition (IMT) in this system. La doping led to an emergence of an intraband response at the expense of the optical excitations across the Mott gap. The intraband response of the metallic compounds was found to be mostly incoherent, indicating a critical role of the electronic correlations. Further we found an abnormal temperature evolution of the low-energy conductivity, which mirrors infrared spectroscopic manifestations of the pseudogap in the high-T_c cuprates. We will compare the infrared response of $(Sr_{1-x}La_x)_2IrO_4$ with that of the cuprates and will discuss the roles of the spin-orbit coupling and the electronic correlations on the electronic structure of the former.

Poster II #33

Dynamical mean-field theory of $LaTiO_3$ /$LaAlO_3$ superlattice

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We performed DFT+DMFT (dynamical mean-field theory) calculation for $LaTiO_3$/$LaAlO_3$ superlattice. We present the electronic and magnetic properties in the space of temperature, interaction strength, and epitaxial strain. In agreement with previous DFT+U result [1], the ferromagnetic-spin and antiferro-orbital order phase is stabilized. It can be understood by superexchange interactions at the strong coupling limit. As temperature increases, the spin order is destroyed while the orbital order still survives due to the lattice effects. Under epitaxial tensile strain, we observed insulator-to- metal transition, while this is not observed in DFT+U.

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Dynamics of single- and multi-vertical-Bloch-line in canted antiferromagnetic rare-earth orthoferrites

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Dynamics of the vertical Bloch line (VBL) in rare-earth orthoferrites ($RFeO_3$) is investigated by using the micromagnetic simulation. We first stabilized the single- and multi-VBL conditions at zero external magnetic field by minimizing magnetic interaction energies including Dzyaloshinskii-Moriya interaction (DMI). Then we examined the VBL dynamics with increasing external magentic field continuously. We found that a velocity of the domain wall (DW) containing VBL is smaller than that of intrinsic DW without VBL. This is because the domain wall mass increases due to the VBL, and hence the DW velocity decreases as a number of the VBL increases. In particular, the DW mass density is inhomogeneous and maximal at the Bloch point, which leads to the DW kink during its propagation. With a further increase of external magnetic field, we found annihilations of the VBL's which are accompanied by aburpt increases of the DW velocity being in good agreement with experimental results. We discussed these processes in terms of a competition between magnetic anisotropy and exchange energies.

Poster II #35

Effect of interactions in the Hofstadter regime of the honeycomb lattice

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The recent realization of Hofstadter butterfly in moire superlattices and realization of the Hofstadter Hamiltonian in the square lattice in cold atom systems motivated this research work. We study the spinless electrons on honeycomb lattice with nearest neighbor hopping and nearest neighbor interactions in presence of magnetic field by using mean field theory. Our main aim in this work is to understand the interaction induced complex phases in detail and study the topology and geometry of the ground state of the system. Further, we study the effect of interaction on the fractal structure of the Hofstadter butterfly. In absence of interactions, the system has two length scales; the magnetic length and the periodicity of the potential i.e. the lattice constant. The interplay of these two length scales leads to the existence of the fractal structure in the energy band gaps. This fractal structure is popularly known as the Hofstadter butterfly. Interactions induce charge ordering which break the translational and rotational symmetry of the system giving rise to anisotropic phases as the ground state for this system. The anisotropy in the particle density can be characterized by quadrupole and dipole moments and the system has complex phases like incompressible nematic and ferrielectric phases as the ground state. These phase transitions are prolific and occur at many values of the flux and particle density. The spontaneous breaking of the translational symmetry introduces a new length scale in the problem. This affects the energy band diagram resulting in the disintegration of the fractal structure of the Hofstadter butterfly. This disintegration increases with increase in the interaction strength. Many of these phase transitions are accompanied with change in the Hall conductivity giving examples of first order topological transitions. Consequently, the disintegration of the Hofstadter butterfly is manifested in the Landau fan diagram also.

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Electronic structure investigation on strongly correlated van der Waals material $NiPS_3$

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Van der Waals (vdW) materials, stacked materials for which constituint layers are bound by electrostatic vdW forces, are getting great attention recently. It has large potential on device industries due to its novel properties and high applicability. On the other hand, strongly correlated electron systems are providing various emergent properties that could be useful when applied on devices. In fact, interesting phenomena such as metal-insulator transition, quantum glass and coherent superconductor are predicted to appear when correlation physics are introduced on graphene, a representative vdW material [1]. Nevertheless, there is little experimental observation for strong interactions in graphene, that may be due to large screening effect [2].

To study correlation effect in vdW crystal, $TMPS_3$ (TM = Mn, Fe, Co, Ni) compounds could be better material platform, as they show long range antiferromagnetic ordering. In order to study electronic structure, we used spectroscopic tools along with DFT+*U* calculations and investigated $NiPS_3$ compound. Indeed, our temperature dependent optical spectrum showed large spectral weight transfer over larger energy range, which is one of characteristics of strong correlation effect. The carrier density showed clear anormaly at Neel temperature, implying close relationship between elecronic and magnetic structure of the system. DFT+*U* calculation verified $NiPS_3$ is charge transfer insulator. Implications on optical conductivity, photoemission spectrum and model calculations will be discussed further.

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Poster II #37

Emergent topological phases in pyrochlore iridates under magnetic field

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Pyrochlore iridates R2Ir2O7 got its attention due to reported remarkable phase transitions by applying magnetic field. Notably, it is acknowledged that Weyl semimetal with antiferromagnetic-ordered state will emerge if R(=Nd) is the element showing obvious magnetism. [111] or [001] direction magnetic field is applied, and the system is investigated through two distinct ways: tight-binding model with Hubbard repulsion, and effective theory for high-symmetry points in Brillouin zone. We show that the magnetic field creates various topological phases in the magnetic-ordered pyrochlore iridates, including "4-pair Weyl semimetal," "3-pair Weyl semimetal," "2-pair Weyl semimetal," "Double Weyl semimetal," and "line node + 1-pair Weyl semimetal," as displayed in the phase diagrams in the paper. This will pave a steady path to find out the phase transition that previously suggested in a number of experiments.

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Generic spin model on a pyrochlore lattice

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Motivated by several pyrochlores, we discuss generic spin model considering nearest and next nearest neighbors. Both Luttinger-Tisza analysis and simulated annealing, we analyze the phase diagram of classical spin model and discuss new types of non-coplanar order induced by anisotropic interactions.

Poster II #39

High tunneling conductance induced by electronic reconstruction at the terrace edges of ultrathin oxide films

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Ultrathin oxide-based heterostructures have attracted considerable interest because of exotic physics and potential device applications. In the few-nanometers-thick oxide films, atomic-scale structural imperfections at the surface and interfaces, albeit adequately investigated, significantly affect the material functionality and device performance. Here, using ultrathin $BaTiO_3$ films as an example, we report an unexpected high tunneling conductance near the one-unit-cell-high terrace edge, which is the most common and inevitable surface imperfection. We observe that the tunneling current near the terrace edges is significantly higher than that within the terrace plateau regions. Spatially-resolved current-voltage spectroscopies and first-principles calculations suggest that surface electronic reconstruction near terrace edges can reduce the effective tunneling barrier width and thus enhance the tunneling conductance. Moreover, we find that this phenomenon could be ubiquitously applicable to other transition-metal-oxides (e.g., $SrTiO_3$). Our work highlights the potential of terrace edge in manipulating transport and electronic properties of ultrathin oxide heterostructures and devices.

Magnetic Anisotropies in Iridates

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Perturbation in electronic structure of strontium iridate is caused by chemical doping, application of magnetic field or pressure that results in a gigantic variety of physical properties. We report the in-plane anisotropy of electronic transport and magnetic properties of strontium iridate (Sr_2IrO_4). The effects of magnetic field(H) and its orientation(θ) on torque measurements(τ) at different temperatures(T) have been carried out in a closed cycle refrigerator (CCR). The τ(H) show a prominent transition from antiferromagnetic(AFM) to weak ferromagnetic(FM) that is attributed to the Dzyaloshinskii-moriya(DM) interaction [1]. Pattern changes from nearly saw-tooth to sinusoidal in τ(θ) take place above FM transition field. The trace of magnetic susceptibility tensor demonstrate the magnetic anisotropy. All the results stipulate the magnetic basal plane anisotropy in Sr_2IrO_4.

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Poster II #41

Polarized optical spectroscopy on anisotropic $BaFe_2Se_3$ single crystal

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The compound of AFe_2Se_3(A=K, Cs, Ba), provides a good playground to understand the iron-based superconductor, since the structure of which is similar to the that of iron-based superconductor. In particular, $BaFe_2Se_3$ (BFS) is known as a quasi-one dimensional spin ladder compound with a needle-like shape. The BFS has been reported as a Mott insulator with charge gap of 0.2 eV. However, due to its 1-D nature, different electronic ground state along different axis has been reported. In order to investigate the this anisotropy behavior, we adopted an optical spectroscopy technique with polarized light. Upon cooling down to 15 K, several localized state were revealed only in b-axis. We will discuss the origin of this 1-D localized state and anisotropic behavior of BFS.

Strong spin-phonon coupling behavior in All-In/All-Out Pyrochlore iridates $R_2Ir_2O_7$ (R = Y, Eu, Sm)

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The 5d transition metal oxides have interesting issues due to their strong-orbit coupling (SOC). It is related to the exotic phenomena including the topological insulator, Weyl semimetal, and etc. Among them, Iridium oxides have appropriate characteristics to research this phenomena. Pyrochlore iridate system has been researched as various aspects and showed the interesting electronic transition phenomena. Recently, similar transition metal oxide, $Cd_2Os_2O_7$ all-in/all-out pyrochlore system, showed the anomaly related to spin-phonon coupling.

We investigated spin-phonon coupling in all-in/all-out pyrochlore iridate system using optical spectroscopy. Pyrochlore iridate $R_2Ir_2O_7$ (R = Y, Eu and Sm) have seven IR-active phonons in far IR regime and show the magnetic transition near T_N of each compounds. Near the transition temperature, we observed clear anomaly in phonon resonance frequencies. Detailed analysis on peak position, scattering rate and spectral weight for each compounds will be discussed.

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Poster II #43

Study of CO oxidation activity on the bimetallic $Pt_3Sn(111)$ surfaces by ARPES

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Pt and Pt alloys have been studied since it shows the best performance as a catalyst of fuel cells. Pt3Sn(111) bulk alloy is particularly interesting, because of its two different surface structure. These two surfaces show huge difference in catalytic activity on CO oxidation reaction. Although the catalytic activity of Pt3Sn(111) with two different surface structure has been studied, the cause of huge catalytic activity difference is not revealed. To understand the catalytic activity difference by observing the electronic structure difference of two surface structure, ARPES has been performed on well ordered Pt3Sn(111) surfaces.

Synthesis and Characterization of the Heavy-Fermion Compound $CePtAl_4Ge_2$

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We report of the synthesis of the Ce-based quaternary compound $CePtAl_4Ge_2$ by Al/Ge self-flux method. It is crystallized in $YNiAl_4Ge_2$-type hexagonal structure (space group *R*-3*m*, #166) with unit cell parameters are a=4.1995(5) Å, c=31.851(7) Å, and γ =120 °, where Ce^{3+} layers and $[PtAl_4Ge_2]^{3-}$ slabs are stacked alternately along the crystallographic *c* axis [1]. Powder X-ray diffraction and energy dispersive X-ray spectroscopy support that $CePtAl_4Ge_2$ ($LaPtAl_4Ge_2$) is in a single phase and homogeneous. Physical properties were investigated by performing electrical resistivity, heat capacity and magnetic susceptibility measurements. The results show some characteristics that are similar to other 1142 compounds [2, 3]. Crystalline electric field and structural factors were suggested to be responsible for anisotropy of the magnetic susceptibility. Below 2.3 K, RKKY interactions between 4*f* and itinerant electrons are important and gives rise to an antiferromagnetically ordered state, which is a rare example in the 1142 germinides. When subjected to magnetic field, the AFM transition temperature is suppressed to zero Kelvin, implying a field-induced quantum critical point in this quaternary compound.

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Poster II #45

Synthesis and Thermal Annealing effects on $BaFe_{2-\delta}Se_3$

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We grew single crystals of $BaFe_{2-\delta}Se_3$ (Ba123) with iron deficiency δ~0.3 by using tellurium-flux method, which revealed semiconducting and spin-glass behavior. By measuring electrical transport, magnetic susceptibility and heat capacity for as-grown and thermal annealed samples, we studied effects of the thermal annealing on the compound. The semiconducting behavior can be interpreted as an activation type at high temperature region and a one-dimensional variable range hopping (VRH) type at low temperature region. The size of activation energy gap (302 meV at 1 bar) gradually decreases with increasing pressure and is suppressed to 110 meV at 2 GPa. The spin-glass behavior which is characterized by the freezing temperature (T_f) is observed near 45 K and 1 kOe and moves to 43 K by applying magnetic field of 10 kOe. When thermally annealed at 700 ˚C for 10 hours, the crystal structure of Ba123 remains same (*Pnma*), but the chemical composition ratio has changed from 1.0:1.7:2.9 to 1.0:1.9:2.7, where the ratio was is normalized by Ba atomic ratio. Thermal annealing introduces an antiferromagnetic phase below 250 K and suppresses the spin-glass temperature to around 10 K. The activation energy gap increases to 253 meV in the annealed compound.

Photon energy dependent circular dichroism in angle-resolved photoemission from Au(111) surface state

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Circular dichroism in angle-resolved photoemission spectroscopy (CD-ARPES) is considered as useful tool for studying the electronic structure of material. There have been various proposals on what the dominating factor of the CD is, including spin, orbital angular momentum (OAM) and the phase of wave function of the initial state as well as the experimental geometry. We performed CD-ARPES with varying incident photon energy ranging from 20eV to 100eV on surface state of Au(111), which is well known for showing Rashba-type spin splitting surface state. Our experimental data show variations of dichroism magnitude as varying incident photon energy. Experimental result and DFT calculation of Au(111) surface state support that CD-ARPES can be used to observe orbital angular momentum(OAM) texture of initial state with insignificant final state effect.

Poster II #47

Observation of magnetoelectric effects in $PbCu_3TeO_7$

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$PbCu_3TeO_7$ is an anisotropic magnetic system which consists of Cu^{2+} (S=1/2) staircase kagome layers and exhibits moderated spin frustration. Herein, we report magnetoelectric (ME) effects of $PbCu_3TeO_7$ single crystals. The ME current and dielectric constant (ε) shows peaks at ~8.2 T at 2 K in which spin flop transition occurs, only for the direction of polarization (P) along a axis and magnetic field (H) along c axis. The pyroelectric current reveals that the H(//c) above 5 T give rise to P below 24 K in which spins order along c direction. Furthermore, the P and ε peak below 24 K becomes larger upon H being increased up to 14 T. A model of magnetic structure of spiral ordering under H(//c) explains the spontaneous P along a axis. Phase diagram is constructed from P, ε, M, χ data which divide the antiferromagnetic (AFM) phase into AFM 1 ($P = 0$) and AFM 2 ($P \neq 0$).

Crystal and electronic structure studies on Bandwidth controlled Mott transition in $NiS_{2-x}Se_x$

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Since the Mott's proposal that an insulating state can appear due to the electron-electron correlation, Mott transition has been one of the most attractive subjects in the field of strongly correlated electron systems. Theoretically, conduction electrons are localized and become a Mott insulator as the Coulomb repulsion becomes dominant over the hopping (that is, bandwidth). However, experimental verification of the theory is not an easy task because band-width controlled Mott transitions often accompany other transitions, such as structural transitions.

$NiS_{2-x}Se_x$ has been known as one of the bandwidth-controlled-Mott-transition (BCMT) material. NiS_2 was known as a charge transfer insulator while another end side $NiSe_2$ is a good metal which is nevertheless iso-valent and iso-structural to NiS_2. Recently, few theoretical papers suggest NiS_2 is not the Mott insulator but the insulator due to the bonding-antibonding splitting in the S - S dimer thus the metal insulator transition is not related to the electron correlation. To reveal the origin of the metal insulator transition, we performed crystal and electronic structure studies on $NiS_{2-x}Se_x$ using X-ray diffraction and angle resolved photoemission spectroscopy. Crystal structural analysis shows atomic displacement within the unit cell as a function of doping and temperature. We observed the distance between Ni and an anion atom jumps across the first order Mott transition while the distance between anion atoms varies monotonically. This result demonstrates that $NiS_{2-x}Se_x$ is an ideal example of BCMT. The electronic structural study corroborates the scenario by showing the bandwidth variation as a function of doping.

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APCTP Asia Pacific Center for Theoretical Physics
CTP Center for Theoretical Physics SEOUL NATIONAL UNIVERSITY
CQMS Center for Quantum Materials & Superconductivity
ibs CCES Center for Correlated Electron Systems
ibs 기초과학연구원 Institute for Basic Science

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