平成 27～31 年度 文部科学省 科学研究費補助金 新学術領域研究（研究領域提案型）領域番号：2704

J-Physics：多極子伝導系の物理
平成 30 年度領域全体会議

平成 30 年 5 月 24 日（木）13:00 ～ 5 月 26 日（土）15:30
東北大学片平さくらホール
（宮城県仙台市青葉区片平 2-1-1）
共催：東北大学金属材料研究所

5 月 24 日（木）

オープニング

13:00 – 13:10	播磨尚朝 （神戸大理）	はじめに

A01 Part1 座長：小林　寿夫

13:10 – 13:35	中辻　　知 （東大物性研）	局在多極子と伝導電子の新しい相関効果
13:35 – 13:55	松林 和幸 （電通大）	非クラマース Pr 系化合物における高圧力で誘起される新奇物性
13:55 – 14:15	菅原 仁 （神戸大院理）	多極子伝導物質の高品質単結晶化と量子振動効果によるフェルミ面の研究
14:15 – 14:35	関山 明 （阪大基礎工）	内殻光電子線二色性=もう一つの角度分解光電子分光による局在 4f 軌道対称性の観測
14:35 – 14:55	星野 晋太郎 （埼玉大理工）	電子面とホール面を持つ相関電子系の近藤効果と超伝導
14:55 – 15:15	井口 敏 （東北大金研）	強相関有機 π-d 電子結合系の電荷-スピン複合物性の解明と探索
15:15 – 15:35	休憩	

C01 Part1 座長：藤 秀樹

15:35 – 16:00	網塚 浩 （北大理）	拡張多極子研究の今後の展開
16:00 – 16:20	本山 岳 （島根大自然科学）	Ce ジグザグ鎖構造を持つ Ce_3TiBi_5 およびその周辺物質における電流誘起磁化現象の探索
16:20 – 16:40	速水 賢 （北大理）	Cross-Correlated Couplings by Toroidal Multipoles through Local Orbital Hybridizations
16:40 – 17:00	Robert Peters （京大理）	Magnetotransport in strongly correlated non-centrosymmetric f-electron materials
17:00 – 17:20	大原 繁男 （名工大院工）	ハニカムおよびジグザグ構造を持つ物質における拡張多極子の研究
17:20 – 17:40	梅尾 和則 （広島大自然セ）	12 GPa までの圧力下比熱測定で視たキラル化合物 $YbNi_3Ga_9$ の圧力誘起による量子臨界現象と磁気秩序相
17:40 – 18:00	阿部 伸行 （東大新領域）	3d 電子系における奇パリティ磁気多極子秩序に由来する電気磁気応答と量子伝導現象

5 月 25 日（金）

C01 Part2 **座長：楠瀬 博明**

9:00 – 9:20	柳澤 達也 （北大理）	電流と格子回転・歪みによる複合共役場を用いた拡張多極子検出の試み
9:20 – 9:40	瀧川 仁 （東大物性研）	スピン軌道結合系および局在多極子系における秩序状態のＮＭＲによる観測
9:40 – 10:00	塩見 雄毅 （東大工）	熱流により誘起された反強磁性マグノンスピン流における奇パリティ多極子効果の開拓
10:00 – 10:20	大串 研也 （東北大理）	奇パリティ多極子秩序系におけるドメイン観察手法の開発と新奇量子伝導の開拓
10:20 – 10:40	大槻 純也 （東北大理）	動的平均場法に基づく多極子秩序の微視的理論
10:40 – 11:00	休憩	

特別セッション **座長：網塚　浩**

「物性若手のためのキャリアデザイン ― 企業で活躍する先輩からのメッセージ」

11:00 – 11:40	四橋 聡史 （パナソニック）	基礎科学から新しい技術開発へのチャレンジ
11:40 – 12:20	角柳 孝輔 （NTT）	NTT 物性科学基礎研究所での超伝導量子回路の研究
12:20 – 13:40	記念撮影・昼食	
13:40 16:10	**ポスターセッション**	

B01 Part1 **座長：神戸　振作**

16:10 – 16:35	青木　大 （東北大金研）	B01 計画研究の今後の方針と展望
16:35 – 16:55	小手川 恒 （神戸大理）	非共型ジグザグ構造における特異な量子相の解明と探索
16:55 – 17:15	橘高 俊一郎 （東大物性研）	磁場角度分解比熱・エントロピー測定からアプローチする多極子伝導系の新奇量子相
17:15 – 17:35	藤本 聡 （阪大基礎工）	ウラン化合物における多重超伝導相の解明と多極子クーパー対の動的電磁応答
17:35 – 17:55	池田 浩章 （立命理工）	遍歴多極子と多極子超伝導体の発展

D01 Part1 **座長：野原　実**

17:55 – 18:15	Kosmas Prassides （WPI-AIMR Tohoku Univ.）	Emergent electronic phenomena in hybrid f-/p-electron molecular materials
18:30 – 20:30	懇談会・ポスター賞表彰（　１階　ラウンジ　）	

5 月 26 日（土）

B01 Part2 **座長：青木　大**

9:00 – 9:20	野尻 浩之 （東北大金研）	URu_2Si_2 の強磁場磁気秩序と磁気相関-磁気相図の確定と対称性破れの検証
9:20 – 9:40	大貫 惇睦 （琉球大理）	立方晶化合物の特異な電子状態
9:40 – 10:00	平井 大悟郎 （東大物性研）	スピン軌道相互作用による不安定性で形成される遍歴多極子秩序
10:00 – 10:20	小林 達生 （岡山大自然）	$Cd_2Re_2O_7$ の高圧下における奇パリティ多極子秩序とパリティゆらぎ超伝導
10:20 – 10:40	休憩	

A01 Part2 **座長：鈴木　通人**

10:40 – 11:00	水戸 毅 （兵庫県立大物質理）	多極子が示す局在―遍歴二重性と秩序の観測
11:00 – 11:20	渡辺 真仁 （九工大基礎科学）	価数転移由来の新規量子現象の理論研究
11:20 – 11:40	椎名 亮輔 （琉球大理）	希土類化合物における軌道依存型混成による電荷秩序と重い電子
11:40 – 12:00	坂井 徹 （兵庫県立大物質理）	フラストレーション系の量子スピンネマティック相
12:00 – 13:20	昼食	

D01 Part2 **座長：鬼丸 孝博**

13:20 – 13:45	野原 実 （岡大基礎研）	D01 計画研究の今後の方針と展望
13:45 – 14:05	岡本 佳比古 （名大院工）	空間反転対称性を「破る」5d 電子系の新物質開拓
14:05 – 14:25	松平 和之 （九工大院工）	幾何学的フラストレート系イリジウム酸化物における新奇物性の研究
14:25 – 14:45	宮坂 茂樹 （阪大院理）	層状・3 次元遷移金属化合物のスピン軌道相互作用由来の異常電子相制御と新規物性探索
14:45 – 15:05	谷垣 勝己 （東北大 AIMR/理物）	遍歴反強磁性物質 $BaMn_2Pn_2$ における電気磁気効果

クロージング

15:05 – 15:30	総括班評価者コメント 領域代表挨拶	

ポスターセッション（5 月 25 日　13:40 - 16:10）

P01：	鶴田 篤史	阪大院基礎工	2 チャンネルアンダーソン格子模型における秩序状態
P02：	植木　輝	弘前大理工	s 波超伝導体の渦糸帯電効果
P03：	渡邉　光	京大理	多極子秩序の群論的分類とその応用
P04：	舩島 洋紀	神戸大院理	電子状態と軌道近藤効果の発現機構の理論的研究
P05：	有田 亮太郎	東大工	反強磁性体における大きな磁気光学カー効果に対するクラスター多極子理論
P06：	柳　有起	明大理工	結晶場一重項-近藤一重項転移によるフェルミ面と多極子応答の変化
P07：	角田 峻太郎	京大理	空間群対称性に守られた非自明超伝導ギャップ構造
P08：	石塚　淳	京大理	非共型結晶における奇パリティ多極子揺らぎと超伝導
P09：	木俣　基	東北大金研	$Cd_2Re_2O_7$ の電流整流効果
P10：	髙力 暁成	北大理	$Ce(Ru_{1-x}Rh_x)_2Al_{10}$ ($x < 0.05$) の電流下磁化測定
P11：	徳永　陽	原研先端研	$CeIn_3$ のパルス強磁場 NMR 研究
P12：	濱本　諭	阪大基礎工	立方晶 PrB_6 の非整合反強磁性相における硬 X 線内殻光電子線二色性の観測
P13：	藤原 秀紀	阪大基礎工	Ground-state 4f symmetry in $CeCu_2Ge_2$ probed by soft x-ray absorption and hard x-ray photoemission spectroscopy
P14：	佐藤 芳樹	東北大工	$CeIr_3$ 単結晶の超伝導特性と上部臨界磁場の研究
P15：	山田 武見	東理大理工	RB_6 系の電子状態の有効ワニエ模型による解析
P16：	工藤 慎也	岩手大院理工	希土類モノプニクタイド HoSb の超音波計測とトポロジー
P17：	中西 良樹	岩手大理工	$EuRh_2Si_2$ の超音波計測と弾性特性
P18：	日高 宏之	北大理	MBe_{13} 系における低温 X 線結晶構造解析
P19：	木村 憲彰	東北大院理	反対称スピン軌道相互作用によって分裂した Yb_4Sb_3 のフェルミ面
P20：	鬼丸 孝博	広大先端	立方晶 $PrNi_4Mg$ の非磁性基底二重項
P21：	山本 将隆	北大理	$TbNiC_2$ における磁化反転異常
P22：	金井 惟奈	阪大基礎工	内殻光電子スペクトル線二色性による強相関 Sm 化合物における 4f 軌道対称性の観測
P23：	本間 佳哉	東北大金研	^{151}Eu Mössbauer Spectroscopy of Chiral Antiffermagnet EuPtSi
P24：	中村 翔太	名工大院工	局所的反転対称性のない $YbNi_{1.8}Si_{3.2}$ の重い電子状態
P25：	小林 寿夫	兵県大物質理	放射光 ^{174}Yb メスバウアー分光法による $YbAlB_4$ の研究
P26：	三宅 和正	阪大先端強磁場	α-$YbAl_{0.986}Fe_{0.014}B_4$ における μSR 緩和率の異常な温度依存性の理論
P27：	川崎 優介	岩手大院理工	籠状物質 PrV_2Al_{20} の磁場誘起量子臨界性
P28：	飯塚 優人	新潟大院自然	第一原理計算に基づく 1-2-20 系の四極子秩序
P29：	中村 一翔	岩手大院理工	籠状物質 $SmPt_2Cd_{20}$ の超音波計測と弾性特性
P30：	奥山 大輔	東北大多元	$PrTr_2Al_{20}$ (Tr = Ti, V) の中性子散乱及び放射光回折による磁性及び結晶構造の研究
P31：	酒井 明人	東大物性研	Multipole order and non-Fermi liquid in quadrupole Kondo lattice PrV_2Al_{20}
P32：	藤　秀樹	神戸大院理	単結晶 UNi_4B の NMR による構造解析
P33：	田端 千紘	KEK 物構研	トロイダル秩序物質 UNi_4B の単結晶構造解析
P34：	播磨 尚朝	神戸大院理	UNi_4B の常磁性電子状態

P35：野間 雄一朗　神戸大院理　強磁性超伝導体 UGe_2 の圧力下における磁気揺らぎの異方性

P36：仲村　愛　東北大金研　トリウム化合物の単結晶育成とドハース・ファンアルフェン効果の研究

P37：Arvind Maurya 東北大金研　Heavy electronic states and spin splitting in $U_3Ni_3Sn_4$

P38：北野 晴久　青学大理工　Fe(Se,Te)単結晶における固有ジョセフソン接合的挙動の電気化学的制御

P39：工藤 一貴　岡大基礎研　Superconductivity in hexagonal BaPtAs and BaPtSb with an ordered honeycomb network

P40：小林 夏野　岡大基礎研　Superconductivity in trilayer (PbSe)n($TiSe_2$)m misfit compound

P41：高橋 武士　岡大　ラーベス相 Au 化合物の超伝導

P42：星　和久　首都大院理　BiS_2 系超伝導体の硫黄同位体効果検証に向けた物質開発

P43：桑田 祥希　神戸大院理　$Ru_{1-x}Rh_xAs$ の超伝導相に対する ^{75}As-NQR

P44：曽我部 遼太　首都大理　高エントロピー合金型ブロック層をもつ BiS_2 系層状化合物の合成

P45：今井　丈　岩手大院理工　$Rh_{17}S_{15}$ の PPMS を用いた超伝導転移近傍の超音波吸収計測

P46：山川 洋一　名大理　鉄系超伝導体における四重極揺らぎと超伝導の理論研究

P47：細井　優　阪大基礎工　$FeSe_{1-x}S_x$ 超伝導体におけるネマティック量子臨界点

P48：肥後 友也　東大物性研　ワイル反強磁性体 Mn_3Sn における巨大な磁気光学カー効果と磁気八極子ドメインの直接観察

P49：中尾 裕則　KEK 物構研　マンガン系人工超格子における Mn3d と O2p の電荷変調の共鳴 X 線散乱による研究

P50：中川 剛志　東北大 AIMR　Pressure response of the mixed valence $RE_{2.75}C_{60}$ (RE: Sm, Eu) fullerides studied by Raman spectroscopy

P51：堀金 和正　岡大　メカニカルアロイ法による $Sr_{2-x}La_xIrO_4$ の磁気相図

P52：藤間 友理　東大新領域　極性磁性半導体 GaV_4Se_8 の低温における熱平衡磁気スキルミオン

P53：江見 知俊　東北大院理　空間反転対称性の破れた反強磁性体 $BaMn_2As_2$ における第二高調波発生

P54：小笠原 拓磨　東北大 AIMR/理物　遍歴反強磁性物質 $BaMn_2Bi_2$ における磁気抵抗効果

FY2015～2019 MEXT KAKENHI on Innovative Areas #2704

J-Physics：Physics of Conductive Multipole Systems

FY 2018 Annual Meeting

Thu. May 24, 13:00 ～ Sat. May 26, 15:30
Sakura Hall, Tohoku University
（2-1-1 Katahira, Aoba-ku, Sendai, Miyagi 980-8577 Japan）

May 24（Thu.）

Opening

13:00 – 13:10	Hisatomo Harima *Kobe University*	Opening Remarks

A01 Part1 — Chair: Hisao Kobayashi

13:10 – 13:35	Satoru Nakatsuji *The University of Tokyo*	Novel Correlation Effects between Localized Multipole and Conduction Electrons
13:35 – 13:55	Kazuyuki Matsubayashi *The University of Electro-Communications*	Exotic phenomena induced by pressure in non-Kramers Pr-based comps
13:55 – 14:15	Hitoshi Sugawara *Kobe University*	High quality single-crystallization of conductive multipole materials and study of Fermi surface by quantum oscillation effect
14:15 – 14:35	Akira Sekiyama *Osaka University*	Observation of localized 4f-orbital symmetry by linear dichroism in core-level photoemission equivalent to another type of angle-resolved photoemission
14:35 – 14:55	Shintaro Hoshino *Saitama University*	Kondo effect and superconductivity in correlated electron systems with electron and hole Fermi surfaces
14:55 – 15:15	Satoshi Iguchi *Tohoku University*	Elucidation and exploration of charge-spin complex properties in organic strongly correlated π-d electrons system
15:15 – 15:35	Coffee Break	

C01 Part1 — Chair: Hideki Tou

15:35 – 16:00	Hiroshi Amitsuka *Hokkaido University*	Research Perspectives on the Physics of Augmented Multipoles
16:00 – 16:20	Gaku Motoyama *Shimane University*	Study of a Current induced magnetoelectric effect on Ce_3TiBi_5 with Ce zig-zag chain structure
16:20 – 16:40	Satoru Hayami *Hokkaido University*	Cross-Correlated Couplings by Toroidal Multipoles through Local Orbital Hybridizations
16:40 – 17:00	Robert Peters *Kyoto University*	Magnetotransport in strongly correlated non-centrosymmetric f-electron materials
17:00 – 17:20	Shigeo Ohara *Nagoya Institute of Technology*	Experimental Study of cluster multipole in the crystal with a honeycomb- and zig-zag structure
17:20 – 17:40	Kazunori Umeo *Hiroshima University*	Quantum criticality and pressure-induced magnetic phases in $YbNi_3Ga_9$ with a chiral crystal structure: AC-calorimetric measurements up to 12 Gpa
17:40 – 18:00	Nobuyuki Abe *The University of Tokyo*	Magnetoelectric Response and Quantum Transport Phenomena Generated by Odd Parity Magnetic Multipole Order in 3d Electron Systems

May 25 (Fri.)

C01 Part2 — **Chair: Hiroaki Kusunose**

9:20 – 9:40	Tatsuya Yanagisawa *Hokkaido University*	Test for detection of augmented multipoles using composite field with electric current, lattice rotation and strains
9:20 – 9:40	Masashi Takigawa *The University of Tokyo*	Observation of ordered states in spin-orbit coupled systems and localized multipole systems by NMR
9:40 – 10:00	Yuki Shiomi *The University of Tokyo*	Thermal spin-current phenomena associated with odd-parity multipoles in antiferromagnetic insulators
10:00 – 10:20	Kenya Ohgushi *Tohoku University*	Visualization of magnetic domains and exploration for novel quantum transport phenomena in odd-parity multipole ordered state
10:20 – 10:40	Junya Otsuki *Tohoku University*	Microscopic derivation of multipolar ordering based on dynamical mean-field theory
10:40 – 11:00	Coffee Break	

Invited Session — **Chair: Hiroshi Amitsuka**

"Career Design for Young Researchers in Condensed Matter Science – Message from Seniors in Private Companies"

11:00 – 11:40	Satoshi Yotsuhashi *Panasonic*	Challenge to new technology from basic science
11:40 – 12:20	Kousuke Kakuyanagi *NTT*	Study of superconducting quantum circuits in NTT Basic Research Laboratories
12:20 – 13:40	Group Photo・Lunch	
13:40 – 16:10	**Poster Session**	

B01 Part1 — **Chair: Hiroaki Kusunose**

16:10 – 16:35	Dai Aoki *Tohoku University*	Plan and perspective of B01 group
16:35 – 16:55	Hisashi Kotegawa *Kobe University*	Elucidation and search of exotic quantum phases in non-symmorphic zig-zag structures
16:55 – 17:15	Shunichiro Kittaka *The University of Tokyo*	Novel quantum phases of conductive multipole systems studied by field-angle-resolved measurements of specific heat and entropy
17:15 – 17:35	Satoshi Fujimoto *Osaka University*	Multiple superconducting phases and dynamical electromagnetic responses of multipole Cooper pairs in Uranium-based heavy fermion systems
17:35 – 17:55	Hiroaki Ikeda *Ritsumeikan University*	Progress of itinerant multipole and multipole superconductors

D01 Part1 — **Chair: Minoru Nohara**

17:55 – 18:15	Kosmas Prassides *Tohoku University*	Emergent electronic phenomena in hybrid f-/p-electron molecular materials

18:30 – 20:30 Get-Together and Free Discussion (1st floor, Sakura Hall)

May 26 (Sat.)

B01 Part2 — **Chair: Dai Aoki**

9:00 – 9:20	Hiroyuki Nojiri *Tohoku University*	High Magnetic Field Order and Magnetic Correlation of URu_2Si_2-Verifing Phase Diagram and Symmetry
9:20 – 9:40	Yoshichika Ōnuki *University of the Ryukyus*	Characteristic Electronic States of Cubic Compounds
9:40 – 10:00	Daigoro Hirai *The University of Tokyo*	Itinerant multipolar order in spin-orbit-coupled metals
10:00 – 10:20	Tatsuo C. Kobayashi *Okayama University*	Odd-parity multipole order and parity fluctuation in $Cd_2Re_2O_7$ under high pressure
10:20 – 10:40	Coffee Break	

A01 Part2 — **Chair: Michi-To Suzuki**

10:40 – 11:00	Takeshi Mito *University of Hyogo*	Observations of multipole's order and localized-itinerant duality
11:00 – 11:20	Shinji Watanabe *Kyushu Institute of Technology*	Theoretical study of new quantum phenomena related to valence transition
11:20 – 11:40	Ryousuke Shiina *University of the Ryukyus*	Charge ordering and heavy fermion due to orbital-dependent hybridization in rare-earth compounds
11:40 – 12:00	Toru Sakai *University of Hyogo*	Quantum Spin Nematic Phase of Frustrated Systems
12:00 – 13:20	Lunch	

D01 Part2 — **Chair: Takahiro Onimaru**

13:20 – 13:45	Minoru Nohara *Okayama University*	Plan and perspective of D01 group
13:45 – 14:05	Yoshihiko Okamoto *Nagoya University*	Exploration of Novel 5d Electron Systems "Breaking" Inversion Symmetry
14:05 – 14:25	Kazuyuki Matsuhira *Kyushu Institute of Technology*	Novel phenomena in geometrically frustrated iridium oxides
14:25 – 14:45	Shigeki Miyasaka *Osaka University*	Control of anomalous electronic states related spin-orbit interaction in 2D/3D transition metal compounds
14:45 – 15:05	Katsumi Tanigaki *Tohoku University*	Electromagnetic properties of itinerant antiferro-magnetic $BaMn_2Pn_2$ (Pn = As, Sb, Bi)

Closing

15:05 – 15:30	Advisor's Comments
	Closing Remarks by Area Representative

Poster Session (May 25, 13:40 - 16:10)

P01:	Atsushi Tsuruta *Osaka University*	Ordered states in two channel Anderson lattice model
P02:	Hikaru Ueki *Hirosaki University*	Vortex charging effect in s-wave superconductors
P03:	Hikaru Watanabe *Kyoto University*	Group-theoretical classification of multipole order and its application
P04:	Hiroki Funashima *Kobe University*	Electronic structures suitable for the orbital Kondo effect
P05:	Ryotaro Arita *The University of Tokyo*	Cluster multipole theory for large magneto-optical Kerr effect in antiferromagnets
P06:	Yuki Yanagi *Meiji University*	Change of Fermi surfaces and multipolar response at transition between crystalline electric field and Kondo singlets
P07:	Shuntaro Sumita *Kyoto University*	Unconventional superconducting gap structure protected by space group symmetry
P08:	Jun Ishizuka *Kyoto University*	Odd-parity multipole fluctuation and superconductivity in non-symmorphic crystalline
P09:	Motoi Kimata *Tohoku University*	Current rectification effect in $Cd_2Re_2O_7$
P10:	Akinari Koriki *Hokkaido University*	Magnetization measurement of $Ce(Ru_{1-x}Rh_x)_2Al_{10}$ ($x < 0.05$) under Electric Current
P11:	Yo Tokunaga *Japan Atomic Energy Agency*	Pulsed high-field NMR study on $CeIn_3$
P12:	Satoru Hamamoto *Osaka University*	Linear Dichroism in core level photoemission spectra of cubic PrB6 on the incommensurate antiferromagnetically ordered phase
P13:	Hidenori Fujiwara *Osaka University*	Ground-state 4f symmetry in $CeCu_2Ge_2$ probed by soft x-ray absorption and hard x-ray photoemission spectroscopy
P14:	Yoshiki Sato *Tohoku University*	Superconducting properties and upper critical field study of $CeIr_3$ single crystal
P15:	Takemi Yamada *Tokyo University of Science*	Analysis of electronic states of the rare-earth hexaborides based on the effective Wannier models
P16:	Shinya Kudo *Iwate University*	Ultrasonic measurements on the possible topological system HoSb
P17:	Yoshiki Nakanishi *Iwate University*	Ultrasound investigation of the Eu-based mixed valence system $EuRh_2Si_2$
P18:	Hiroyuki Hidaka *Hokkaido University*	Low-temperature x-ray crystal structure analysis of MBe_{13} system
P19:	Noriaki Kimura *Tohoku University*	Split Fermi Surfaces in Noncentrosymmetric Yb_4Sb_3
P20:	Takahiro Onimaru *Hiroshima University*	Nonmagnetic doublet ground state of a cubic system $PrNi_4Mg$
P21:	Masataka Yamamoto *Hokkaido University*	Peculiar Magnetization Reversal of $TbNiC_2$
P22:	Yuina Kanai *Osaka University*	Ground-state 4f orbital symmetry probed by linear dichroism in core-level photoemission spectra of strongly correlated Sm compounds
P23:	Yoshiya Homma *Tohoku University*	^{151}Eu Mössbauer Spectroscopy of Chiral Antiffermagnet EuPtSi
P24:	Shota Nakamura *Nagoya Institute of Technology*	Heavy fermion state of $YbNi_{1.8}Si_{3.2}$ without local inversion symmetry
P25:	Hisao Kobayashi *University of Hyogo*	Synchrotron-radiation-based ^{174}Yb Mössbauer spectroscopic studies on $YbAlB_4$

P26: Kazumasa Miyake, *Osaka University* — Theory for anomalous temperature dependence of relaxation rate measured by μSR in α-$YbAl_{0.986}Fe_{0.014}B_4$

P27: Yusuke Kawasaki, *Iwate University* — Quantum criticality induced by magnetic field in the cage compound PrV_2Al_{20}

P28: Yuto Iizuka, *Niigata University* — Quadrupole order in 1-2-20 system based on first-principles calculations

P29: Kazuto Nakamura, *Iwate University* — Ultrasonic measurements on the cage compound $SmPt_2Cd_{20}$

P30: Daisuke Okuyama, *Tohoku University* — Neutron scattering and synchrotron x-ray diffraction study on $PrTr_2Al_{20}$ (Tr = Ti, V)

P31: Akito Sakai, *The University of Tokyo* — Multipole order and non-Fermi liquid in quadrupole Kondo lattice PrV_2Al_{20}

P32: Hideki Tou, *Kobe University* — NMR structural analysis in single crystal UNi_4B

P33: Chihiro Tabata, *KEK IMSS* — X-ray Crystal Structure Analysis of Toroidally Ordered System UNi_4B

P34: Hisatomo Harima, *Kobe University* — Paramagnetic electronic structure of UNi_4B

P35: Yuichiro Noma, *Kobe University* — Anisotropy of magnetic fluctuations under pressures in ferromagnetic superconductor UGe_2

P36: Ai Nakamura, *Tohoku University* — Study of Single Crystal Growth and de Haas—van Alphen Effect in Thorium Compounds

P37: Arvind Maurya, *Tohoku University* — Heavy electronic states and spin splitting in $U_3Ni_3Sn_4$

P38: Haruhisa Kitano, *Aokyama Gakuin University* — Electrochemical control of hysteretic current-voltage characteristics in single-crystal of Fe(Se,Te) superconductor

P39: Kazutaka Kudo, *Okayama University* — Superconductivity in hexagonal BaPtAs and BaPtSb with an ordered honeycomb network

P40: Kaya Kobayashi, *Okayama University* — Superconductivity in trilayer $(PbSe)_n(TiSe_2)_m$ misfit compound

P41: Takeshi Takahashi, *Okayama University* — Superconductivity in Laves structured Au compound

P42: Kazuhisa Hoshi, *Tokyo Metropolitan University* — Material development for the sulfur isotope effect in the BiS_2-based superconductor

P43: Yoshiki Kuwata, *Kobe University* — ^{75}As-NQR investigation of superconducting phase in $Ru_{1-x}Rh_xAs$

P44: Ryota Sogabe, *Tokyo Metropolitan University* — Synthesis of BiS_2-based layered superconductors with high-entropy-alloy-type blocking layers

P45: Zyo Imai, *Iwate University* — Ultrasound attenuation around Tc of $Rh_{17}S_{15}$

P46: Youichi Yamakawa, *Nagoya University* — Theoretical study on quadrupole fluctuation and superconductivity in Fe-based superconductors

P47: Suguru Hosoi, *Osaka University* — Nematic Quantum Critical Point in $FeSe_{1-x}S_x$ superconductors

P48: Tomoya Higo, *The University of Tokyo* — Large magneto-optical Kerr effect and imaging of magnetic octupole domains in the antiferromagnetic Weyl metal Mn_3Sn

P49: Hironori Nakao, *KEK IMSS* — Charge disproportionation of Mn3d and O2p in $(LaMnO_3)_2(SrMnO_3)_2$ superlattices studied by a resonant x-ray scattering

P50: Nakagawa Takeshi, *Tohoku University* — Pressure response of the mixed valence $RE_{2.75}C_{60}$ (RE: Sm, Eu) fullerides studied by Raman spectroscopy

P51: Kazumasa Horigane, *Okayama University* — Magnetic phase diagram of $Sr_{2-x}La_xIrO_4$ synthesized by mechanical alloying

P52: Yuri Fujima
The University of Tokyo
Thermodynamically stable magnetic skyrmion at low temperatures in a polar magnetic semiconductor GaV_4Se_8

P53: Kazutoshi Emi
Tohoku University
Second Harmonic Generation of noncentrosymmetric antiferromagnet $BaMn_2As_2$

P54: Takuma Ogasawara
Tohoku University
Giant negative magnetoresistance of itinerant $BaMn_2Bi_2$

Novel effects due to the correlation between localized multipoles and conduction electrons

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The subject of A01 group is to study the novel quantum phenomena driven by the strong hybridization between localized mulitipoles and conduction electrons. I will review the recent activities made by A01 group during the first three year period. Our study covers not only the atomic multipoles but also the cluster multipoles. Then, we will discuss the future goals and plans for the upcoming two years.

Exotic phenomena induced by pressure in non-Kramers Pr-based compounds

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Since the discovery of non-Kramers Γ_3 doublet ground state in PrT_2X_{20} (T: transition metal, X=Al, Zn) compounds, many interesting phenomena associated with the quadrupolar degrees of freedom have been reported [1-3]. In particular, the strong hybridization between the Γ_3 ground doublet and conduction electrons gives rise to the quadrupolar Kondo effect as well as superconductivity. However, the underlying mechanisms for the appearance of superconductivity and the associated fluctuations remain unclear.

So far, we have studied the effect of pressure on PrT_2Al_{20} (T=Ti, V) and constructed the phase diagrams, mainly based on resistivity measurements. In both compounds, applying pressure suppresses the quadrupole order and the enhancement of superconducting transition temperature near the putative quantum critical point of the quadrupole order. At a critical pressure P_C, where the quadrupole order order disappears, the low-temperature resistivity becomes quite incoherent and the NFL state emerges in wide pressure and field range. In this region, the resistivity curves are shown to collapse onto a single scaling function, as predicted for the quadrupole Kondo lattice model [5]. In the case of $PrTi_2Al_{20}$, we found the striking enhancement of the upper critical field toward $P_C \sim 11$ GPa. The large upper critical field exceeding both Pauli and orbital limits suggests unconventional superconductivity in this compound. In fact, recent theoretical works have shown that unconventional superconductivity such as local nodal Cooper pairs and mass-imbalanced superconductivity can be realized in non-Kramers Γ_3 doublet ground state system [6,7]. During this two-years research project, we will develop specific heat and quantum oscillation measurement system under pressure to shed light on the superconducting properties and the interplay between the quadrupole order and superconductivity.

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High quality single-crystallization of conductive multipole materials and study of Fermi surface by quantum oscillation effect

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Unusual physical properties observed in PrM_2Al$_{20}$ (M = Ti, V) and CeT_2Al$_{10}$ (T = Fe, Ru, Os) have attracted much attention in conductive multipole systems. The former shows the heavy fermion superconductivity in the proximity of multipole (or quadrupole) order, implying that the superconductivity is mediated by the multipolar interaction [1-4]. The latter is classified as Kondo semiconductor exhibiting unusually high antiferromagnetic transition temperatures: CeRu$_2$Al$_{10}$ and CeOs$_2$Al$_{10}$ order at 27 K and 29 K, respectively, while CeFe$_2$Al$_{10}$ shows no magnetic order at low temperatures [5]. For these unusual properties in PrM_2Al$_{20}$ and CeT_2Al$_{10}$, it is suggested that the interaction between the multipole of Pr^{3+}(or Ce^{3+})-ions and conduction electrons plays an important role, and the singularity of electronic state of these materials, such as Fermi surface and energy density of states at Fermi level, should be involved.

The quantum oscillation effects, such as de Haas-van Alphen (dHvA) effect and Shubnikov-de Haas (SdH) effect, are powerful tools to observe the Fermi surface and cyclotron mass. So far, we have succeeded in observing the dHvA effect in PrTi$_2$Al$_{20}$ for the first time and revealed the Fermi surface with highly enhanced effective mass [6]. For CeRu$_2$Al$_{10}$, we have observed the SdH effect and revealed the small Fermi surface suggesting the semi-metallic state at low temperatures [7]. In this project we will extensively continue the high quality single-crystal growth of PrM_2Al$_{20}$ and CeT_2Al$_{10}$ to reveal these electric states. In addition, we will also explore the new materials especially focusing on the crystal structure exhibiting the 4*f*-sites are lacking inversion symmetry. In this talk, the progress of our studies on PrM_2Al$_{20}$ and CeT_2Al$_{10}$ by the quantum oscillation effects and the future plans will be presented.

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Observation of localized 4f-orbital symmetry by linear dichroism in core-level photoemission equivalent to another type of angle-resolved photoemission

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Localized 4f-orbital symmetry is crucial for many exotic phenomena induced by multipoles in rare-earth-based strongly correlated electron systems. Recently, we have developed the technique for uniquely determining the 4f-orbital symmetry by linear dichroism (LD) in ***angle-resolved*** core-level photoemission [1,2]. Figure 1 shows the x-ray optics for our polarized hard x-ray photoemission (HAXPES) installed by us, which has been described elsewhere [2]. By using this technique, we have so far revealed the crystal-field 4f ground-state symmetry of tetragonal $YbCu_2Si_2$ and $YbRh_2Si_2$ [1], and cubic YbB_{12} [3]. It has also been clarified that LDs reflecting the anisotropic charge distributions are seen for a tetragonal Sm compound [4] and Ce compounds [5]. Further, LDs have also been systematically observed for Pr compounds under cubic symmetry as shown in Fig. 2. We have established that LD-HAXPES can be applicable for many rare-earth compounds.

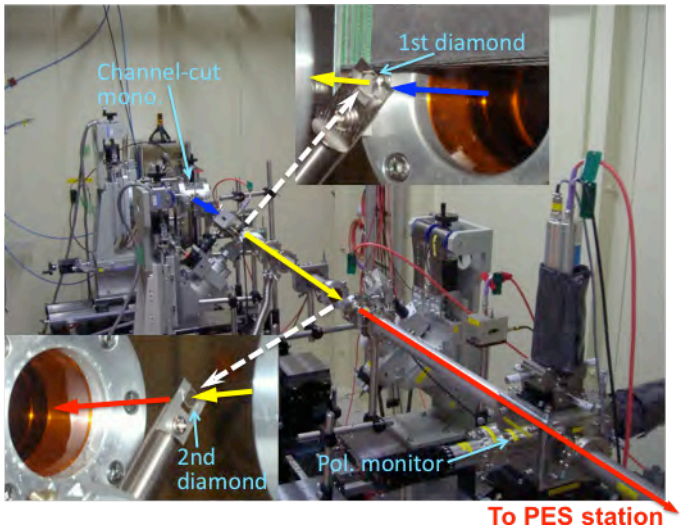

Fig. 1 Photograph of beamline optics in SPring-8 BL19LXU for polarized hard x-ray photoemission spectroscopy. The insets show an x-ray phase retarder by using two diamond plates. Circularly polarized x-ray is obtained after the first diamond from horizontally polarized synchrotron radiation, and vertically polarized x-ray is obtained after the second diamond.

Our work has been performed under collaboration with T. Onimaru (Hiroshima U), H. Hidaka, H. Amitsuka (Hokkaido U), T. Ebihara (Shizuoka U), Y. Onuki (U Ryukyus), F. Iga (Ibaraki U), Y. Saitoh (SPring-8, JAEA), Y. Nakatani, K. Yamagami, H. Aratani, S. Fujioka, M. Kawada, S. Takana, and T. Kashiuchi (Osaka U).

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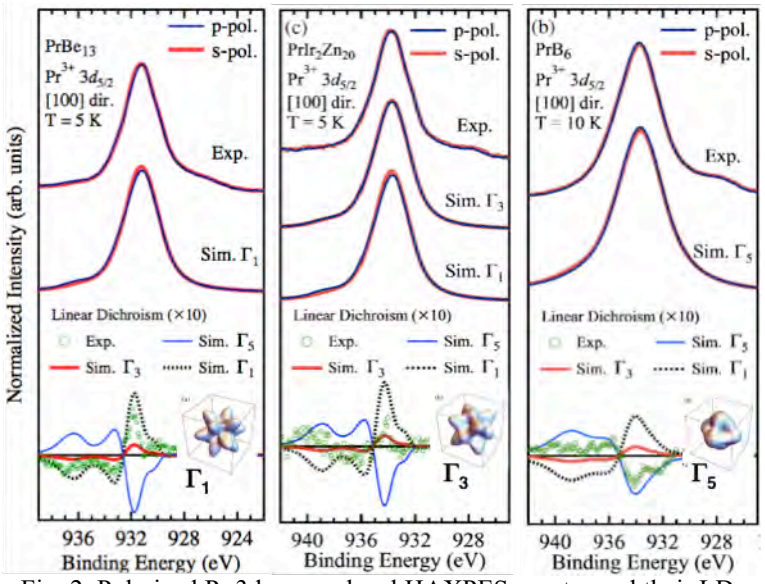

Fig. 2 Polarized Pr $3d_{5/2}$ core-level HAXPES spectra and their LDs of $PrBe_{13}$, $PrIr_2Zn_{20}$, and PrB_6 in paramagnetic phases along the [100] direction, which are compared with the theoretical simulations by ion models under crystalline electric fields.

Kondo effect and superconductivity in correlated systems with electron and hole Fermi surfaces

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One of the fundamental phenomena in condensed matter physics is the spontaneous symmetry breaking. In electronic systems, the degrees of freedom that electrons possess are spatially aligned driven by the interactions to show the long-ranged ordering, and its control has been an important issue in designing the useful devices. In addition to standard magnetic and orbital ordered states, the excitonic insulator has recently attracting attention, which is an electronic ordering that utilizes the degrees of freedom composed of electron and hole Fermi surfaces usually realized in compensated metals [1]. This has been interpreted based on the weak-coupling limit as a particle-hole transformed analog of the BCS superconducting state.

Another interesting issue in this context is the interplay between the above electron/hole Fermi surfaces and localized spins, which is typically realized as Kondo lattices in f-electron materials. When the semimetallic degrees of freedom are viewed as channel, the system is effectively regarded as the two-channel Kondo system [2]. We have clarified in the previous studies the basic properties of ordering phenomena in the two-channel Kondo lattice, and found a variety of symmetry-broken states including s-wave superconducting states [3] plus their physical mean-field picture [4]. Since the superconducting states are both gapless and gapful depending on the situation, it is also interesting in connection with the recently identified full-gap superconductivity in $CeCu_2Si_2$ [5]. An extension of the work of multi-channel Kondo systems to the semi-metallic Kondo lattice will open a new route to the interesting behaviours in heavy-electron materials.

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Elucidation and exploration of charge-spin complex properties in organic strongly correlated π-d electrons system

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Organic molecular conductors represented as (BEDT-TTF)$_2X$ (X^- = monovalent anion) have been intensively studied because of the appearance of wide variety of electronic properties such as metal-insulator transition, magnetic, ferroelectric, and superconducting transitions, etc. To understand the electron correlations of them, Mott and charge ordering transitions have been thoroughly investigated. Many of (BEDT-TTF)$_2X$ crystals have two-dimensional structure, where BEDT-TTF molecular layers attributing to the electron conduction are separated each other by monovalent anion (X) layers (see Fig.1 as an example). Thus, two-dimensional conduction layer often appears. Because of the charge neutrality, a BEDT-TTF molecule has 0.5 hole on average. The hole carriers partially fill a band made of the π-orbitals of BEDT-TTF. Without dimerization, the BEDT-TTF molecular band is typically quarter-filled and often the system shows a charge-ordered state [1].

Recently, we have found a BEDT-TTF based new compound, α''-(BEFT-TTF)$_2$Rb$_{1.2}$Co(SCN)$_4$ (α''-RbCo, Fig. 1), showing metal-insulator transition similarly to the other α'' crystals [2]. α'' is the name of phase which represents the arrangement of BEDT-TTF molecule in the layers. The metal-insulator transition occurs at about 100 K. There are two remarkable features of α''-RbCo: First is that magnetic exchange interactions between the Co^{2+} and the π-electron spins are expected. Second, the electron band filling in the system deviates from 3/4. Actual stoichiometry of α''-RbCo is Rb$_{1.2}$Co. Therefore, 0.1 electrons are doped by in a BEDT-TTF molecule on average. The study of (BEDT-TTF)$_2X$ salts with these (complex) features are rather unique in this field.

To clarify the metal-insulator transition in α''-RbCo, we obtained the optical conductivity down to 5 K (Fig. 2). We found a splitting of the infrared active ν_{27} mode below around 100 K indicating the transition to a charge ordered phase. Another anomaly at about 40 K was observed in in-plane spectra and the other properties related to magnetism, probably due to a magnetic transition of the BEDT-TTF spins. Below 40 K we observed anomalies in the magnetocapacitance effects, indicating a coupling between the π-electrons and Co^{2+} spins, as well as curious magneto-transport in the metallic phase. By elucidating these phenomena, we will explore new charge-spin complex phenomena in (BEDT-TTF)$_2X$ systems.

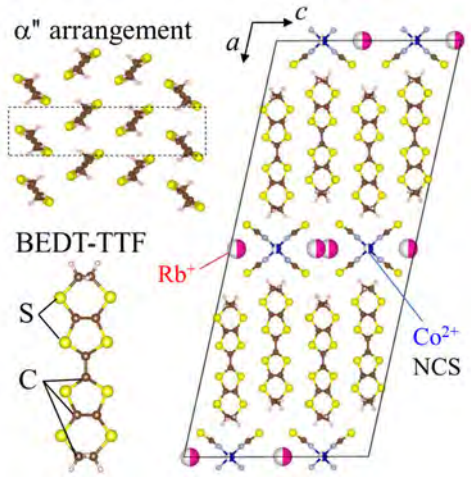

Fig. 1. Crystal structure of α''-RbCo.

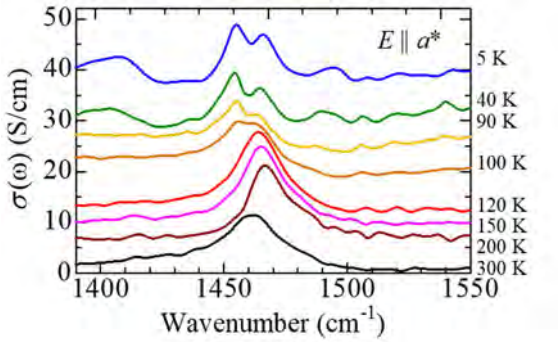

Fig. 2. Optical conductivity of α''-RbCo. The spectra are shifted for clarity. Splitting of the peak at around 1460 cm^{-1} is seen.

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Research Perspectives on the Physics of Augmented Multipoles

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The Planned-Research Group C01 has been conducting experimental and theoretical studies on static and dynamical properties of "augmented multipoles", which have been introduced and developed in the J-Physics project as extension of "traditional multipoles" formed by a single orbit on a single ion. One of the most important advances made in the first-half term of the project would be the theoretical formularization of the concept of the augmented multipoles, where they are clearly defined, consisting of two types of extension: "cluster multipoles" formed from multi-site spins or charges, and "hybrid multipoles" formed from multi-orbits around an ion [1]. The investigation of a variety of cross correlations among magnetic, electric and elastic degrees or freedom driven by emergence of the cluster multipoles have now been intensively conducted not only in C01 but also in other groups. As materials investigated in this line so far, UNi_4B [2-4], α-$Cu_2V_2O_7$ [5,6], $Co_4Nb_2O_9$ [7,8], $BaMn_2As_2$ [9], Mn_3Sn [10], $ErNi_3Ga_9$ [11], StPtAs [12] are exemplified. In the second-half term of the project, we will expand and deepen the studies of this trend for further understanding the basics properties of the cluster multipoles and exploring their new functions in view of new application. We are also planning to make a careful search for the substances where hybrid multipoles emerge as hidden order parameters. It will be very important to establish a typical example of such systems, demonstrating the direct observation of hybrid orbitals as well as precise structural refinement using resonant and non-resonant synchrotron X-ray diffraction [13]. We will also work actively to make significant progress in the development of new materials that provide a playground with augmented multipoles particularly involving spontaneous parity violation. Establishment of a noble technique for controlling chirality would be one of the major challenges we focus on [14].

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Study of a Current induced magnetoelectric effect on Ce_3TiBi_5 with Ce zig-zag chain structure

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We have succeeded in growing the single crystals of hexagonal $P6_3/mcm$ Ce_3TiBi_5 by the Bi self-flux method [1]. Moreover the crystal structure of the newly discovered compound U_3TiBi_9 was determined to be hexagonal $P6_3/m$ [2]. It shows a very similar crystal shape between the both single crystals of Ce_3TiBi_5 and U_3TiBi_9. The both crystal structures are hexagonal, although the space groups are different from each other, as shown in Fig. 1. They have same Bi face-sharing octahedral chains centred of a Ti atom, however a Bi single chain or a Bi triangle prism lies between the three octahedral chains of Ce_3TiBi_5 and U_3TiBi_9, respectively. The change from the single chain to the triangle prism additionally results in a slight octahedral chain's rotation about the c-axis [1, 2]. The sites of Ce and U of both compounds are not located on the inversion center, especially Ce atoms form a zig-zag chain structure. Measurements of electrical resistivity, magnetic susceptibility, and specific heat have been made on the both compounds. The results indicate that both Ce_3TiBi_5 and U_3TiBi_9 are new compounds with an antiferromagnetic ordering temperature T_N of 5.0 and 31.5 K, respectively. Therefore both compounds are one of the good candidates for a study of a current induced magnetoelectric effect.

In order to measure a current induced magnetoelectric effect, we have improved two measurement probes. The first one is a measuring rod to enable to apply current to a sample for magnetization measurement using a commercial magnetometer system. The second one is a measurement system for magnetic field using a Hall device. Although any proof of the EM effect on Ce_3TiBi_5 have not observed yet, some hints of the accuracy improvement were obtained.

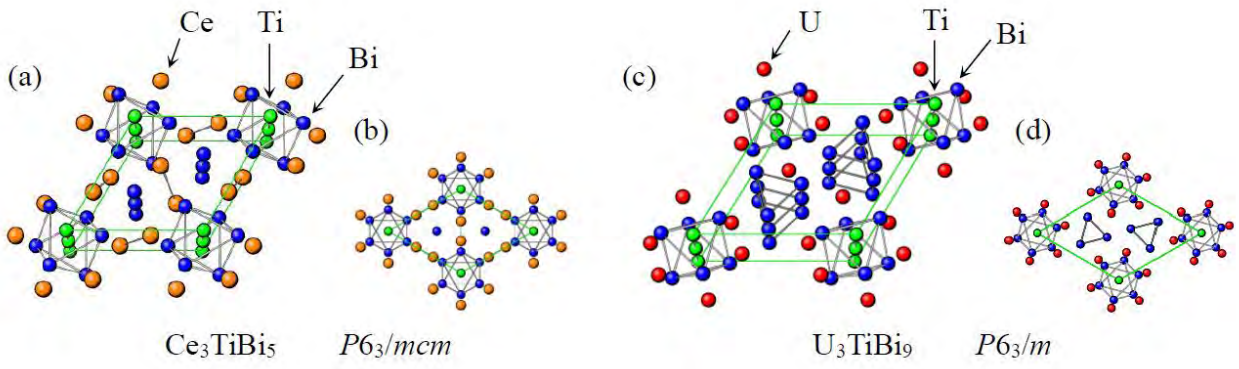

Fig. 1. Crystal structure of (a), (b) Ce_3TiBi_5 and (c), (d) U_3TiBi_9.

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Cross-Correlated Couplings by Toroidal Multipoles through Local Orbital Hybridizations

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The multipole moments are used to characterize electric charge and current distributions, whose concept has been widely developed in various fields of physics at different length scale, such as classical electrodynamics and nuclear and molecular physics. In condensed matter physics, they have been recognized as important quantities to describe multiple degrees of freedom in electrons, e.g., charge, spin, and orbital, from the microscopic viewpoint [1-3]. Under the space-time inversion group, there are four types of fundamental multipoles according to their spatial inversion and time-reversal properties: electric (E: polar/true tensor with time-reversal even), magnetic (M: axial/pseudo tensor with time-reversal odd), magnetic toroidal (MT: polar/true tensor with time-reversal odd), and electric toroidal (ET: axial/pseudo tensor with time-reversal even) multipoles. Among the toroidal multipoles, the MT dipole has been extensively investigated in the field of multiferroics due to its potential role for exotic magneto-electric phenomena [4]. Such a MT dipole is often recognized as a vortex-type magnetic structure over several atomic sites. However, it can be emergent even at each atomic site from the viewpoint of the space-time symmetry. Thus, it is desirable to obtain quantum-mechanical operator expressions of toroidal multipoles, in contrast to previous discussions as classical electromagnetic quantities [5]. Once we obtain such expressions, we can clarify when it can be a primary order parameter characterizing thermodynamic phases in condensed matter.

In the present study, we discuss a general microscopic formalism to describe not only MT but also ET multipoles [6]. By starting the classical description in the expansion of electromagnetic scalar and vector potentials, and using the mutual correspondence among four multipoles, we derive the quantum-mechanical operator expressions of both ET and MT multipoles in addiction to conventional E and M multipoles. We demonstrate that the ET and MT multipole degrees of freedom can be active in the Hilbert space spanned by orbitals with different azimuthal quantum number, e.g., *s*-*d*, *p*-*d*, and *d*-*f* hybrid orbitals. We also demonstrate emergent cross-correlated couplings, such as magneto-electric and magneto(electro)-elastic couplings, once an ET or MT multipole ordering occurs. Moreover, we discuss a classification of MT and ET multipoles in real and momentum spaces under crystallographic point groups in order to understand physical phenomena in a more systematic way with respect to multipole terminology [7]. This work has been collaborated with Hiroaki Kusunose (Meiji University), Yuki Yanagi (Meiji University), and Megumi Yatsushiro (Hokkaido University).

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Magnetotransport in strongly correlated non-centrosymmetric f-electron materials

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The combination of strong spin orbit interaction (SOI) and strong correlations has recently aroused great interest. In heavy elements, SOI can become large and strongly affects low temperature properties resulting in fascinating phenomena such as the Quantum Spin Hall effect or the magnetoelectric effect. On the other hand, in materials with partially filled f-electron orbitals, strong electron correlations can commonly be observed, which results in intriguing physics such as magnetism, quantum criticality, and unconventional superconductivity. The combination of both, strong correlations and strong spin orbit interaction, can thus be expected to result in completely novel phenomena such as spin-orbit assisted Mott insulators, spin liquids, correlated topological insulators.

This project aims at theoretically understanding the interplay of strong correlations and strong spin-orbit interaction, particularly in the situations of f-electron materials with broken inversion symmetry, which leads to the asymmetric SOI, such as the Rashba interaction. Examples of these materials are $CePt_3Si$, $CeRhSi_3$ and $CeIrSi_3$ which even become superconducting at very low temperatures. Besides these noncentrosymmetric f-electron materials, recently, superlattices, in which the inversion symmetry is broken at the interface, have been proposed as a new platform for utilizing the combination of strong Rashba SOI and strong correlations.

Due to the combination of strong Rashba interaction and strong Coulomb correlations spin-dependent transport, fascinating ordered states, and exotic higher angular momentum Kondo liquids can be expected to occur in these systems. Besides introducing these topics in this talk, I will give a concrete example for interesting physics arising from the interplay of Rashba SOI and strong electron correlations, namely I will show that correlations can strongly enhance the Edelstein effect in f-electron materials with broken inversion symmetry [1]. The scattering between itinerant conduction electrons and localized f electrons at temperatures above the Kondo temperature can lead to a momentum dependent spin polarization of the conduction electrons. Most remarkably, because of an absence of cancellation effects, this spin polarization results in a strongly enhanced Edelstein magnetoelectric effect. This example demonstrates the potential for interesting phenomena inherent in strongly correlated materials with strong Rashba spin orbit interaction.

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Experimental Study of Cluster Multipole in the Crystal with a Honeycomb and a Zig-zag Structure

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Cluster multipole is a new concept of the spatially extended multipole over several atomic sites [1-3]. Antiferromagnetic order on a locally non-centrosymmetric structure such as a zig-zag chain or a honeycomb plane, can be seen as the odd-parity cluster multipole order. When the odd-parity cluster multipole forms ferroic order, peculiar physical properties, such as current-induced magnetization, are caused by the asymmetric spin-orbit interaction [4].

To study the physics caused by the cluster multipole order, we have grown the single crystals of ternary rare-earth intermetallic compounds RNi$_3$Al$_9$, RNi$_3$Ga$_9$, R_2Pt$_6$Ga$_{15}$, and R_2T_3Ga$_9$ (R=rare-earth element, T=Rh, Pd, and Ir). In these crystals, the rare-earth ion forms a honeycomb structure and thus the inversion symmetry is broken at the rare-earth site. Furthermore, the different magnetic structures appear at low temperature for each compound. Therefore, these compounds are good candidates for studying the cluster multipole order. We have investigated the current-induced magnetization for these compounds. Until now, it is found that *Ising*-like antiferromagnet of ErNi$_3$Ga$_9$ [5] shows the current-induced magnetization below the magnetic ordering temperature of 6.4 K.

We have also tried to grow a new heavy-fermion (HF) ytterbium-based compound with a locally non-centrosymmetric structure. We searched a ternary compound of ytterbium-transition metal-silicon and obtained YbNi$_2$Si$_3$ and Yb$_2$Rh$_3$Si$_5$. In both compounds, the inversion symmetry is broken locally at Yb-site. YbNi$_2$Si$_3$ crystallizes in tetragonal ScNi$_2$Si$_3$-type structure with a space group of $I$4/mmm (#123, D_{4h}). This crystal structure is similar to that of antiferromagnetic HF superconductor of YbRh$_2$Si$_2$ [6] and non-centrosymmetric pressure-induced superconductor of CeIrSi$_3$ [7]. Yb$_2$Rh$_3$Si$_5$ belongs to the monoclinic system with a space group of $C$2/c (#15, C_{2h}). In Yb$_2$Rh$_3$Si$_5$, Yb-ions form a zig-zag chain. We found that both compounds are in HF state at low temperature by the specific heat and magnetization measurements. Further study on the ground state of these new Yb-based compounds is being undertaken.

We will address the crystal structure and the magnetic properties for materials mentioned above and describe our research plan.

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Quantum criticality and pressure-induced magnetic phases in $YbNi_3Ga_9$ with a chiral crystal structure: AC-calorimetric measurements up to 12 GPa

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The Yb-based compounds $YbNi_3X_9$ (X = Al, Ga) crystallize in the trigonal $ErNi_3Al_9$-type structure with a chiral space group $R32$, making them unique candidates for systems exhibiting chiral magnetic structures as well as quantum critical phenomena [1, 2]. $YbNi_3Al_9$ undergoes an antiferromagnetic (AFM) transition at $T_M = 3.4$ K [3]. By substituting 6% of Cu for Ni, a chiral soliton lattice (CSL) is realized under magnetic fields B applied parallel to the a-axis [1, 4, 5].

$YbNi_3Ga_9$, on the other hand, is an intermediate-valence system under ambient pressure [3]. We expect a pressure-induced magnetic order to occur in this compound. Indeed, an AFM order above $P_c = 9$ GPa was inferred from the electrical resistivity $\rho(T)$ and AC magnetic susceptibility measurements [2]. At P_c, $\rho(T)$ exhibits a linear-T dependence, i.e. non-Fermi liquid behavior.

In this work, we have investigated the quantum critical behavior and antiferromagnetic order in the chiral magnet $YbNi_3Ga_9$ using AC-calorimetric measurements under pressures P up to 12 GPa [6]. Thereby, magnetic fields B were applied parallel and perpendicular to the c axis. As shown in Fig. 1, the specific heat C divided by temperature T, C/T, dramatically increases with applying pressure. At 8.6 GPa $\cong P_c$, C/T exhibits $-\ln T$ dependence for $2 < T < 9$ K. At $T < 1.5$K, C/T is saturated to a constant value 1 J/K^{2}mol, i.e., Fermi-liquid behavior. At $P = 9.3$ GPa $> P_c$, a broad maximum in C/T appears at 1.6 K, reflecting the AFM order. With increasing P further, the maximum shifts to higher temperatures and becomes a sharp λ-type peak at 5 K for $P \geq 11$ GPa. By using the data of $C(T, P)$ obtained under $B \perp c$ and $B // c$, we have constructed B-T phase diagrams at each P value as shown in Fig. 2. The results at $P \geq 11$ GPa have another field-induced ordered (FIOP) phase denoted by phase II appearing only for $B \perp c$. We discuss the origin of the FIOP in relation to the CSL for $Yb(Ni_{1-x}Cu_x)_3Al_9$ and A-phase for MnSi [7] and EuPtSi [8].

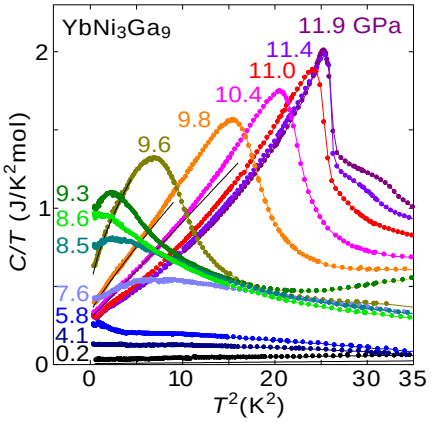

Fig. 1. Specific heat divided by temperature C/T vs T^2 for $YbNi_3Ga_9$ under various pressures up to 12 GPa.

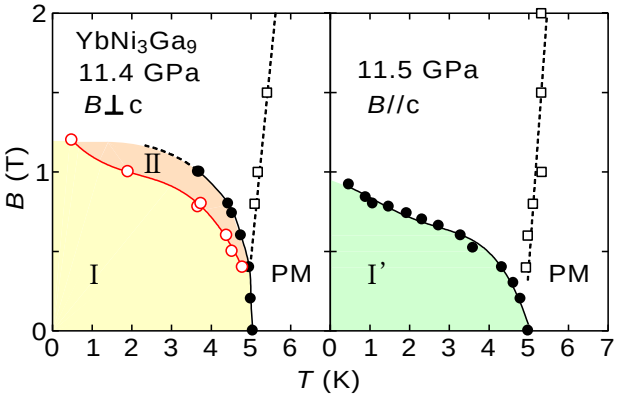

Fig. 2. B-T phase diagrams for $B \perp c$ at 11.4 GPa and $B // c$ at 11.5 GPa determined by specific-heat measurements.

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Magnetoelectric Response and Quantum Transport Phenomena Generated by Odd Parity Magnetic Multipole Order in 3d Electron Systems

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The properties and functions of materials are closely related to symmetry. For example, breaking of spatial inversion symmetry causes ferroelectricity and chirality. Time-reversal symmetry breaking appears as ferromagnetism. These functions are widely used as a basic principle of various electronic and storage devices. Whereas global symmetry is broken ferromagnets and ferroelectrics, recent studies also pointed out the importance of local symmetry breaking. Typical examples of local inversion symmetry breaking are surfaces and interfaces. For example, spin splitting of bands due to the Rashba effect [1] and non-collinear magnetism derived from Dzyaloshinskii-Moriya interaction are observed at the interface of thin films [2]. Even in bulk, the importance of odd parity multipoles accompanied by local inversion symmetry breaking has been pointed out for the tetrahedral crystal field, zigzag structure, honeycomb structure and so on [3,4]. In these cases, it is expected that ferroic order of odd parity magnetic multipole and toroidal moment will be realized, and novel physical phenomena like magnetoelectric coupling will emerge.

In this research, we aim to develop novel physical properties derived from odd parity magnetic multipole order in 3d electron systems, such as optical magnetoelectric responses [5-7] of odd parity magnetic multipole ordered state and quantum transport phenomenon accompanied by local inversion symmetry breaking [8].

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Test for Detection of Augmented Multipoles using Composite Field with Electric Current, Lattice Rotation and Strains

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Odd-parity magnetic multipole is activated through an antisymmetric spin-orbit coupling, which emerges not only in a globally noncentrosymmetric system but also when a local space-inversion symmetry is broken due to charge and/or magnetic order. In the present research project, we will test for the detection of the odd-parity magnetic multipoles, whose dynamic response will couple to the lattice strain or rotation induced by acoustic wave using ultrasound, especially for magnetic quadrupole moment, magnetic hexadecapole moment and magnetic toroidal moment with certain symmetry, which have not been detected by regular experimental method thus far. We use external electric current or magnetic field combined with strain field induced by ultrasound in order to detect the dynamical response generated by such "hidden" odd-parity multipoles.

$BaMn_2As_2$ is one of the candidate materials for the present research. This compound is a parent compound of Iron-pnictide superconductors and has the space group of I4/ mmm (No. 139) in the paramagnetic phase. This structure is same as the one in the well known 1-2-2 systems including URu_2Si_2, which undergoes an enigmatic phase transition so called 'hidden order' and unconventional superconducting state. On the other hand, $BaMn_2As_2$ undergoes G-type antiferro magnetic (AFM) transition below T_N = 625 K (Fig. 1: Left) [1]. Resent theoretical investigation gave us a new point of view that the G-type AFM state can be considered as occurring a B_{1u}-type hybrid-magnetic-hexadecapolar-ordering state (or cluster-magnetic-quadrupolar ordering state) accompanied by simultaneous time-reversal and space-inversion symmetry breaking [2]. In this theory, the following 'magnetopiezoelectric' effect is also predicted; the electric field along the *c* axis will induce the electric quadrupole moment in the *ab* plane, which leads to the tetragonal-orthorhombic lattice distortion through electron-lattice couplings (as shown in the Fig. 1: Right). The ultrasonic measurement under electric current is one of the very easy but quite sensitive methods to detect such (might be tiny) spontaneous strain in the metallic compound with possible domains as strain susceptibility. We will also test the above assumptions on the other candidate compounds such as $Ba_{1-x}K_xMn_2As_2$, DyB_2C_2, UIr_2Ge_2 and URu_2Si_2 with the collaboration of Prof. K. Ohgushi, Dr. R. Watanuki, and Prof. H. Amitsuka.

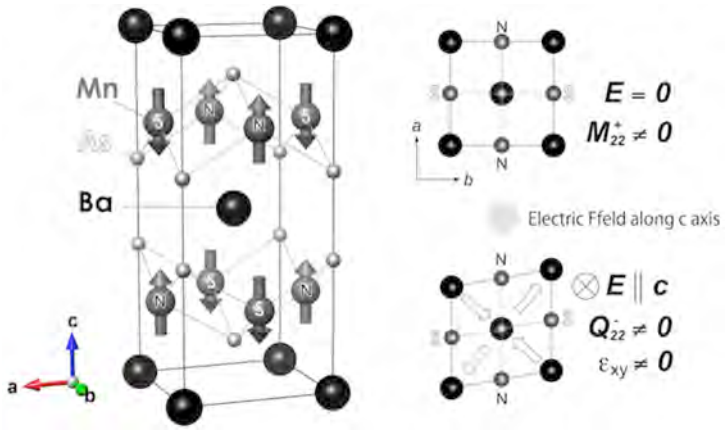

Fig. 1. Left: The crystallographic and the magnetic structures of $BaMn_2As_2$.
Right: Schematic illustration of the current-induced structural transition.

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Exploring Novel Orders in Spin-Orbit Coupled and Localized Multipole Systems by NMR

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In this study, we plan to investigate two distinct but perhaps closely related problems by NMR. The first one is novel electronic orders in spin-orbit coupled metals which spontaneously break inversion symmetry. Recent theories [1,2] predict that the spin-orbit coupling in inversion symmetric metals generates anisotropic spin-spin interaction, which can cause Fermi surface instability towards parity breaking but time-reversal conserving phases. A remarkable feature of such ordered phases is the characteristic spin texture in the momentum space. $Cd_2Re_2O_7$ is a candidate material, which shows two-step parity breaking structural transitions at 200 K and 120 K, which are proposed to correspond to multipolar phases [1].

Some time ago, we performed Re-NQR and Cd-NMR experiments in $Cd_2Re_2O_7$ and detected symmetry lowering two-step transitions [3,4], most notably, strong discontinuity in the direction of the principal axis (fig. 1) and sing change of the asymmetry parameter of the Knight shift across the lower temperature transition (fig. 2). Although the spin texture in momentum space cannot be detected directly by NMR because the time reversal symmetry is preserved, such feature may be a signature of strong influence of multipolar order. We first plan to repeat such measurements on recently grown crystals with much higher quality, then, to characterize various distinct phases that appear under high pressure including superconducting phases with enhanced T_c and H_{c2} [5].

The second problem is the multipolar order in Pr based compounds PrT_2Al_{20} (T=Ti, V), which have non-magnetic Γ_3 crystal field ground state. Although here multipoles are basically localized, we expect strong p-f hybridization in the V material or Ti material at high pressure may lead to phenomena associated with itinerant multipoles. We plan to perform Al-NMR to determine the symmetry of the order parameters and their fluctuations.

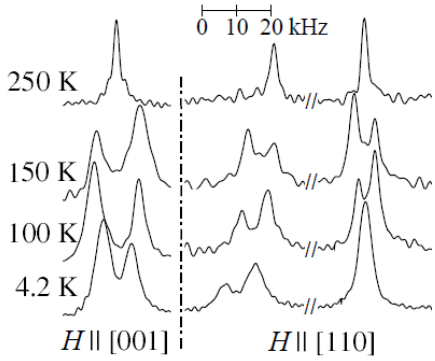

fig. 1. Cd-NMR spectra in Cd2Re2O7 at

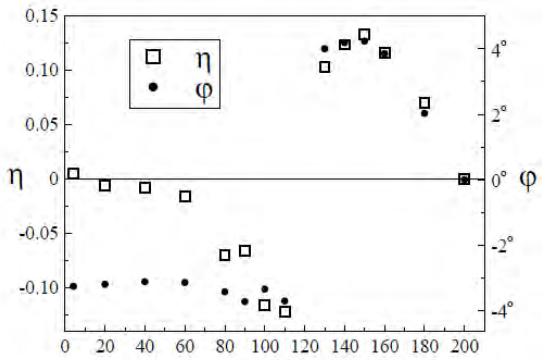

fig. 2. Temperature dependences of the direction of the principal axis (φ) and asymmetry parameter (η) of the Cd Knight shift..

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Thermal spin-current phenomena associated with odd-parity multipoles in antiferromagnetic insulators

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In this presentation, we report thermal generation effects of spin currents in two antiferromagnetic materials with zigzag spin-chain structures: $MnPS_3$ [1, 2] and α-$Cu_2V_2O_7$ [2, 3].

For a layered antiferromagnetic insulator $MnPS_3$ in contact with two Pt strips, we observed signature of a magnon Nernst effect, an antiferromagnetic analogue of the magnon Hall effect in ferromagnetic insulators [1]. Thermoelectric voltage measured in the Pt strips grown on the $MnPS_3$ single crystals was found to exhibit nonmonotonic temperature dependence at low temperatures, which is unlikely to be explained by electronic origins in Pt but can be ascribed to the inverse spin Hall voltage induced by the magnon Nernst effect.

For α-$Cu_2V_2O_7$/Pt bilayers, we performed the measurement of the longitudinal spin Seebeck effect [3]. The antiferromagnetic spin Seebeck effect was clearly observed and its temperature and magnetic-field dependences were analysed by a magnon spin current theory. The numerical calculation of spin Seebeck voltages using magnetic parameters of α-$Cu_2V_2O_7$ determined by previous neutron scattering studies reveals that the antiferromagnetic spin Seebeck effect for α-$Cu_2V_2O_7$/Pt is consistent with the reported magnon dispersions.

Very recently, we theoretically studied a nonreciprical spin Seebeck effect, i.e. nonreciprocal spin transport generated by a temperature gradient in $MnPS_3$ and α-$Cu_2V_2O_7$ [2]. For α-$Cu_2V_2O_7$, we found that a nonlinear spin Seebeck signal appears as an even function of magnetic field, whereas the conventional linear spin Seebeck signal is odd (Fig. 1). Especially at zero magnetic field, the system even exhibits a perfect nonreciprocal spin transport. In contrast, the nonlinear spin Seebeck effect in $MnPS_3$ is odd for magnetic field similarly to the linear spin Seebeck effect, but exhibits a strong directional dependence not expected in high-symmetric magnets, as shown in Fig. 1.

This work was done in collaboration with R. Takashima, D. Okuyama, G. Gitgeatpong, P. Piyawongwatthana, K. Matan, T. J. Sato, and E. Saitoh.

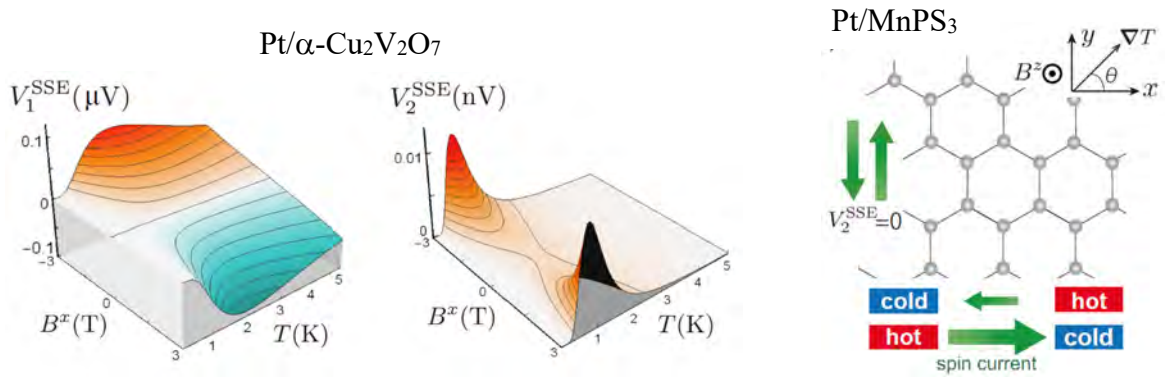

Fig. 1. (Left) Linear and nonlinear spin Seebeck effect in Pt/α-$Cu_2V_2O_7$. (Right) Directional dependence of nonlinear spin Seebeck effect in Pt/$MnPS_3$. [2]

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Visualization of Magnetic Domains and Exploration for Novel Quantum Transport Phenomena in Odd-parity Multipole Ordered State

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All the iron-based superconductors identified so far share a square lattice composed of iron atoms as a common feature. In copper-based high-T_c materials, the superconducting phase emerges not only in square-lattice structures but also in ladder structures, which give nice hints for elucidating the microscopic mechanism of the superconductivity. Therefore, novel Fe-based superconductors without a square lattice had been highly expected. We have been investigating an iron-based ladder material $BaFe_2S_3$, a Mott insulator with striped-type magnetic ordering below 120 K [1, 2]. We found that, on the application of pressure, this compound exhibits a metal–insulator transition at about 11 GPa, followed by the appearance of superconductivity below T_c = 24 K.

On the other hand, iron-based ladder materials are considered to be a nice platform for exploring odd-parity multipole ordered states. Actually, a high- T_c multiferroic state was theoretically predicted in $BaFe_2Se_3$ [3]. Here, I will be talking about our efforts in searching multiferroic phase in this material by using the second-harmonic generation spectroscopy.

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Microscopic derivation of multipolar ordering based on dynamical mean-field theory

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Phase transitions observed in f-electron materials are well explained by multipole theory based on localized picture. A mean-field treatment of an effective multipolar interactions further yields behaviors of static physical quantities that appear in a symmetry-broken state. There are, however, some exceptions which cannot be understood by the ordinary multipole theory, such as URu_2Si_2 and $PrFe_4P_{12}$. Those materials imply a need for expanding the concept of multipole beyond localized picture and a simple mean-field theory.

In this project, we address multipolar ordering in microscopic point of view. Starting from first principles Hamiltonian including detailed atomic structures and energy dispersions, we derive multipolar fluctuations in realistic materials. We will thus achieve

(i) quantitative descriptions of multipolar ordering in realistic materials, and
(ii) possibility of unconventional multipolar ordering which involves conduction electrons as well as localized f-electrons.

Methods

For first-principles calculations of electronic structures in strongly correlated materials, much effort has been made in developing dynamical mean-field theory on top of density functional theory (DFT+DMFT) [1,2]. We apply this framework to calculations of momentum-dependent multipolar susceptibilities. In practice, it is quite hard to solve the equation that involves the vertex part of the two-particle correlations. We will obtain a reasonable solution by developing a method and approximation that works in a specific situation.

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Plan and perspective of B01 group

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We show our plan and perspective of B01 group for next two years in J-Physics project. In my group, IMR and CEA, we focus on the Fermi surface instabilities induced by the itinerant multipole, which might be related to the so-called “Pomeranchuk instabilities” or Nematic state. High quality single crystals are inevitably important. We plan to develop some new crystal growth systems, such as RF furnace, compact SSE, dynamical pumping annealing system, etc. The target materials are ferromagnetic superconductors, UGe2, URhGe, UCoGe, new compounds without inversion symmetry, materials with chiral structure, cage structure, zigzag chain, etc. Thorium compounds without inversion symmetry are also an important target in order to study the fermiology focusing on the strong spin-orbit interaction. Another important aspect is the FIB process for the electrical resistivity measurements for magnetoelectric effect, SdH effect, symmetry breaking, from the view point of topological materials physics and engineering, using micrometer size samples.

Elucidation and search of exotic quantum phases in non-symmorphic zig-zag structures

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Zig-zag structures often provide fascinating quantum phases in condensed matter physics. For instance, ferromagnetic superconductivity is realized in U-zig-zag structures in UGe_2, URhGe, and UCoGe.[1-3] Another example is pressure-induced superconductivity in CrAs, which is a first magnetic Cr-based superconductor.[4-5] Besides superconductivity, RuAs shows an interesting metal-insulator transition.[6] As shown in Fig.1, URhGe, UCoGe, CrAs, and RuAs possess similar zig-zag structures of the crystals in non-symmorphic space group *Pnma*. The atomic sites such as U or Cr lack the local inversion symmetry and the inversion center is in the middle of the two sites. Interesting hypothesis is that such zig-zag structures favor the exotic quantum phases, but the details are unsolved.

A first purpose in our research is an elucidation of the quantum phase of some zig-zag materials to find a common key ingredient to induce the exotic phase transition. The current targets are CrAs (3*d* system), RuAs (4*d*), and UGe_2 (5*f*). Figure 2 shows the pressure-temperature phase diagram of CrAs. The helimagnetic (HM) phase is easily suppressed by applying pressure, and then superconductivity (SC) with T_c = 2.2 K appears. In the paramagnetic (PM) region, a close relationship between the magnetic fluctuation and superconductivity is observed.[7] Recent NMR measurements suggest that the magnetic correlation in the PM state contains the non-negligible ferromagnetic (Q ~ 0) component. To reveal a parity and a gap function of the superconducting phase, we plan to measure NQR/NMR under pressure by using a dilution refrigerator.

A second purpose in our research is a discovery of new exotic quantum phase by synthesizing high-quality crystals and applying pressure. The targets are non-symmorphic crystals with zig-zag structures, which extend from 3*d* electron systems to 5*f* electron systems.

In the presentation, we will show the current status of the research of CrAs, recent results on RuAs,[8] and some results on an exploring research for new quantum phase.

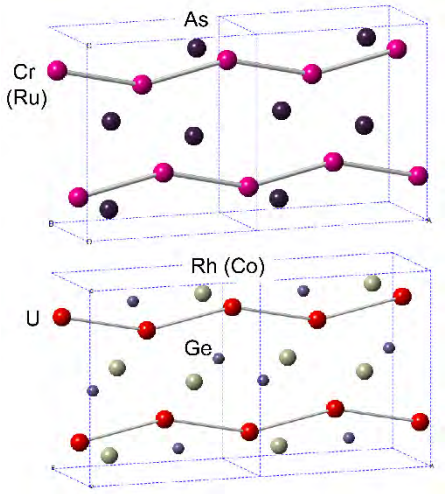

Fig.1: Similarity in crystal structures between CrAs（RuAs）and URhGe（UCoGe）in the *Pnma* space group

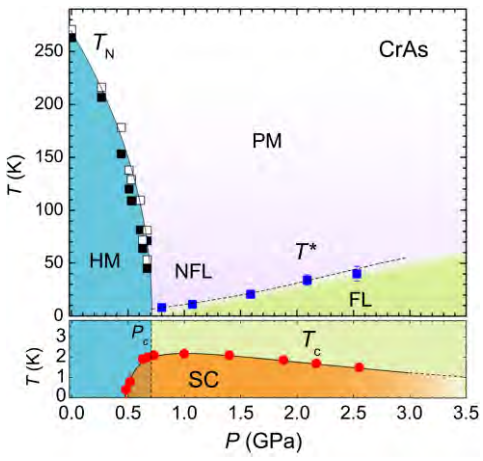

Fig.2: Pressure-temperature phase diagram of CrAs

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Novel quantum phases of conductive multipole systems studied by field-angle-resolved measurements of specific heat and entropy

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A variety of exotic phenomena such as magnetic order, multipole order, spin frustration, unconventional superconductivity, and quantum criticality, have been discovered in condensed matters. In order to understand the physics behind them, the effect of the applied magnetic-field orientation is sometimes very important. For instance, the field-angle dependence of quasiparticle excitations in nodal superconductors is useful to elucidate the location of nodes in the superconducting gap [1], which provides crucial hints to resolve exotic pairing mechanisms.

Recently, we have developed a new technique to study the anisotropy of novel quantum phases. By this technique, we can measure the thermodynamic entropy S and the specific heat C as a function of a magnetic field angle ϕ_H, with high resolution [2]. It takes advantage of the rotational magnetocaloric effect which is a temperature change in the response to an adiabatic change of a magnetic-field orientation. The reliability of this method has been established by investigating the field-angle dependence of the entropy for the spin-ice compound $Dy_2Ti_2O_7$.

Because the entropy and the specific heat change sensitively at a phase transition, we have applied this technique to the study of the field-orientation dependence of a ferroquadrupole (FQ) order in $PrTi_2Al_{20}$ [3]. We found that a magnetic field of larger than 1 T induces a FQ moment in the paramagnetic state when the magnetic field is tilted away from the <111> direction. In other words, the FQ transition at $T_Q \sim 2$ K is rigid only when the magnetic field is applied precisely along the <111> direction, and it becomes crossover above 1 T in other field orientations. The low-temperature entropy, however, becomes small only when the magnetic field is applied near the <001> direction, indicating that the Zeeman effect hardly changes the energy gap between the ground and first-excited states in H // <110>, as well as in H // <111>, at least below 5 T. These experimental facts bring important information for constructing the FQ model for $PrTi_2Al_{20}$.

These works have been done in collaboration with T. Sakakibara, S. Nakamura, H. Kadowaki, H. Takatsu, T. Taniguchi, M. Takigawa, M. Tsujimoto, A. Sakai, Y. Matsumoto, and S. Nakatsuji.

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Multiple superconducting phases in Uranium-based heavy fermion systems and electrodynamics of multipole Cooper pairs

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We investigate multiple superconducting (SC) phases of the Uranium-based heavy fermion systems, $U_{1-x}Th_x\ Be_{13}$ and UCoGe, and novel electromagnetic and transport properties characterizing these phases. Both of these materials are putative odd-parity superconductors.

It is known that for $U_{1-x}Th_x\ Be_{13}$, at least three distinct superconducting phases are realized as the concentration of Th and temperature are varied [1]. According to the recent specific heat measurement combined with a group-theoretical argument [2], there are two promising scenarios for the multiple SC phases; (i) E_u representation scenario, (ii) accidental degeneracy scenario based on Au representation. In the former scenario, the three phases are (a) nematic SC state, which is fully gapped, and also a class DIII topological SC state protected by time-reversal symmetry, (b) nematic SC state, which has point nodes, and also a Dirac SC state, and (c) non-unitary SC state with broken time-reversal symmetry, which has point nodes carrying nonzero monopole charges in the momentum space, and hence, is a Weyl SC state. On the other hand, in the latter scenario, the three phases are (a) A_{1u} pairing state which is also a topological SC state, (b) A_{2u} pairing state which is also a Dirac SC state with point nodes, and (c) non-unitary state, which is fully-gapped, or has accidental nodes, and is neither topological nor Weyl SC state. An important question is how one can determine the SC phase diagram, utilizing unique features of these phases. To answer this question, we explore distinct phenomena characterizing these phases. For instance, in the non-unitary Weyl SC state of the E_u scenario, various novel phenomena arising from Weyl quasiparticles can occur; e.g. negative magnetoresistivity of thermal current associated with chiral anomaly, the anomalous thermal Hall effect, and Landau quantization due to chiral magnetic fields synthesized by using lattice strain. Furthermore, for both the E_u and A_u scenarios, the SC phases with multi-component order-parameters can give rise to low-energy collective modes, which can be detected via electromagnetic wave absorption. We investigate the possibility of determining the phase diagram by using these effects.

For UCoGe, which is a ferromagnetic superconductor characterized by a non-unitary pairing state, various experimental studies suggest the possibility of the phase transition of the SC state induced by applied pressure or applied magnetic fields [3][4][5]. In fact, it is theoretically predicted that an applied magnetic field parallel to b-axis, for which remarkable enhancement of upper critical fields is observed [4], the phase transition from the non-unitary state to a unitary pairing state occurs, which is a result of magnetic criticality caused by the interplay between the applied magnetic field and a DM-type interaction caused by a zigzag crystal structure of this material [6]. We explore novel phenomena characterizing this phase transition, particularly, focusing on the role of multipole degrees of freedom of Cooper pairs composed of j=5/2 electrons.

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Progress on Itinerant multipole and multipole superconductors

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The concept of multipole has become increasingly important. So far, we have studied multipole ordering/fluctuations and unconventional superconductivity emerging in heavy-electron materials, based on the first-principles approach; For examples, rank-5 E^- ordering in URu_2Si_2 [1], d_{x2-y2}-wave pairing state in $CeCoIn_5$ [2], $s_\pm$ -wave pairing state mediated by octupole fluctuations in $CeCu_2Si_2$ [3], and the E_{2u} gap structure in UPt_3 [4]. Then, we have realized that in the multi-orbital superconductors, the superconducting gap functions can be classified like multipole moments. We summarized in tables possible gap functions in typical crystal structures [5]. In this work, we found that (i) *s*-wave pairing states in multi-orbital superconductors with orbital degeneracy can possess not symmetry-protected but inevitable line nodes or gap minima. (ii) Anisotropic pairing state can appear even within the BCS approximation of local interactions. As a prototypical example of the case (i), we studied a gap anisotropy in the BiS_2 layered superconductors in a multi-orbital attractive Hubbard model [6]. For the case (ii), we considered a possible local pairing in an f^2 crystalline electric field ground state [7]. Furthermore, we have indicated the presence of symmetry-protected line nodes in non-symmorphic magnetic group, like UPd_2Al_3 and UCoGe [8]. However, these interesting scenarios have been studied based on simple models and/or simple DFT calculations. In heavy-electron systems, the effect of electron correlations is important. Therefore, we here study the electronic structures in such heavy-electron systems based on the recently-developed DFT+DMFT code.

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Emergent electronic phenomena in hybrid f-/p-electron molecular materials

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The electronic properties of the rare earth elements are typically dominated by the +3 oxidation state. Well-established exceptions include Ce, Sm, Eu, Tm, and Yb compounds, in which the +4 or +2 oxidation states can be also stabilized. Of particular interest in such circumstances are selected rare earth systems (Kondo insulators, heavy fermions) for which the 4*f* levels lie close to the Fermi level, E_F and may exhibit mixed valence phenomena. Unambiguous signatures of electronically-driven valence changes with changes in external stimuli (temperature, pressure) are found for instance in the variation of the elastic, electronic, and magnetic properties of such mixed valence solids.

In this contribution, we will focus on emergent electronic phenomena in the family of hybrid *f*-/*p*-electron molecular materials we have been researching to-date within J-Physics. In particular, we have synthesized and researched new families of molecular-based strongly correlated *f*-electron fullerides in which the presence of the electronically-active C_{60} anions is combined with mixed configuration rare earth ions potentially leading to properties intrinsically unattainable in other systems currently available. Strong correlations dominate the electronic properties of both the rare-earth cation and the C_{60} anion sublattices. To-date our work has unambiguously led to the authentication – by both structural (synchrotron X-ray diffraction) and spectroscopic (Raman spectroscopy, synchrotron X-ray absorption spectroscopy, resonant inelastic X-ray scattering) techniques at ambient and elevated pressures – of the occurrence of valence transitions with novel characteristics arising from the simultaneous presence of the electronically-active C_{60} sublattice. In addition, we have been also developing by both isovalent and aliovalent metal a family of mixed valence materials with chemically (and potentially physically) quasi-continuously tunable valence transitions.

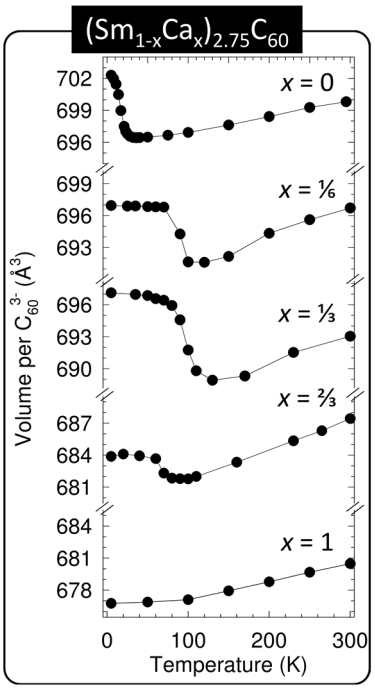

Fig. 1. Temperature-induced valence transitions in $Sm_{2.75-x}Ca_xC_{60}$ probed by synchrotron XRD.

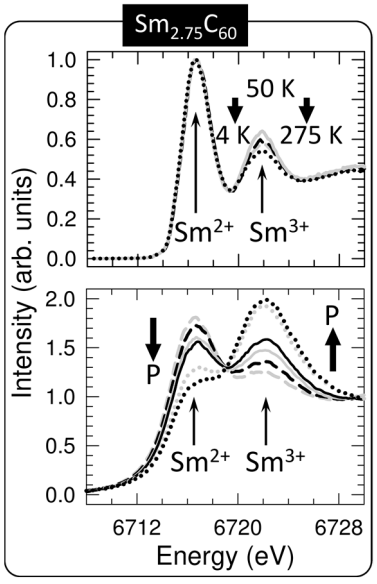

Fig. 2. Temperature- and pressure-induced valence transitions in $Sm_{2.75}C_{60}$ probed by XAS

High Magnetic Field Ordered Phase and Correlation in URu_2Si_2 - Elucidating Magnetic Phase Diagram and Symmetry Breaking

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We have investigated the high field phases of URu_2Si_2 by means of neutron diffraction and X-ray spectroscopies. The compound shows a magnetic ordered when the hidden order is collapsed by strong magnetic fields. There are four magnetic phases including forced paramagnetic phase and the nature of these phases should relate to their counterpart-the hidden order. Therefor, the determination of the magnetic structures of the field induced phases has the primary importance. We have made a series of neutron diffraction experiments on high magnetic fields for URu_2Si_2 and found that the phase II and III are both spin density wave like incommensurate magnetic phases with q~[0.6 0 0][1]. On the other hand, we have identified that the magnetic wave vector is commensurate [2/3, 0, 0] for Rh 4 % [2]. More recently, the identical wave vector is observed for higher Rh doping[3] and the equivalence between the (1 0 0) and (0 1 0) was also confirmed. In 2% Rh doping, we confirmed that the commensurate modulation is absent. These findings show that there is a phase transition along with the Rh doping around the concentration between 2 % and 4 %. It is noteworthy that the hidden order phase disappears by increasing Rh doping at around this concentration. In another word, the electronic state gives rise to the hidden order causes the incommensurate magnetic phases. When the hidden order disappears for the change of the electronic state, the commensurate order set in. It means that change of the electronic states between higher and lower Rh doped regimes is the key to cause the hidden order. If we could call this transition is the quantum phase transition, there should be a quantum critical point at around 3 % Rh doping. More recently, we have measure pure URu_2Si_2 in spallation neutron source. Although the statistic is not enough to give a conclusive remark, the result shows a possibility of 2nd component of the magnetic modulation. It is not clear at present, if it comes from the slightly different magnetic wave vector along (1 0 0) and (0 1 0) or the small splitting of the incommensurate peak.

The aim of this project is to elucidate the possibility of the splitting of magnetic wave vector and the symmetry breaking-symmetry lowering in high field phase. For this purpose, we will continue the present white beam Laue diffraction in high magnetic fields for pure URu_2Si_2. The determination of the incommensurate wave vector of 2% sample will be also performed. For the lattice part, we have investigated the tetragonal crystal structure in the hidden order phase. The existence of the lattice distortion and symmetry breaking in high field phase will be examined by the combination of a pulsed magnetic field and an X-ray free electron laser. The combination could detect peaks as week as 10^{-6} of the fundamental peak at very high magnetic fields. These investigations will establish the high field phase diagrams of pure and Rh doped URu_2Si_2.

We have also examined the magnetic field induced meta-magnetic transition(crossover) in $CeRu_2Si_2$ and $CeRh_2Si_2$ by means of X-ray circular magnetic dichroism(XMCD) to understand the difference between U and Ce systems. In XMCD of $CeRh_2Si_2$ with antiferromagnetic order at 38 K, a clear increase of XMCD signal of $4f_1$ state is found for high magnetic fields. We also found an additional $4f_0$ signal, which shows the admixture of itinerant state in ordered system of $CeRh_2Si_2$. By the success of recent technical development, we could measure XMCD at low temperature of 2 K, where the thermal effect on the meta-magnetic transition is much suppressed. We successfully found the induced enhancement of XMCD signal at the meta-magnetic transition. The investigation will continue to examine the nature of the field induced transition in Ce compounds.

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Characteristic Electronic States in Cubic Compounds

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We will study the characteristic electronic states of cubic compounds and their related compounds, as follows:

1) Ullmannite-type compounds EuPtSi, EuPtGe, EuPdSi, EuIrP
2) CaPtSi, SrPtSi, BaPtSi, BaPtGe
3) non-centrosymmetric tetragonal compounds LaPtSi, CePtSi
4) $Th_3Ni_3Sn_4$
5) P and Sn based compounds MnP, Mn_2P, Cu_3P, Sn_4P_3

The ullmannite(NiSbS)-type compounds of categories (1) and (2) crystallize in the cubic chiral structure ($P2_13$, No. 198), which is the same as the crystal structure of MnSi with the skyrmion structure. EuPtSi orders antiferromagnetically below a low Néel temperature T_N = 4.05K. The magnetization at 2 K for the magnetic field along the [111] direction indicates two metamagnetic transitions at H_{A1} = 9.2 kOe and H_{A2} = 13.8 kOe and saturates above H_c = 26.6 kOe. The present magnetic phase between H_{A1} and H_{A2} is closed in the (H, T) phase and is observed in a wide temperature range from 3.6 to 0.5 K. In this magnetic phase, we found giant additional Hall resistivity and magnetoresistance [1, 2]. We will continue the single crystal growth and the study of the other ullmannite-type compounds.

The similar compounds of LaPtSi and CePtSi are not cubic but tetragonal, with the noncentrosymmetric crystal structure. We will grow single crystals by means of the Bridgman method using the Mo crucible, as in EuPtSi and study the superconducting and magnetic properties.

$Th_3Ni_3Sn_4$ in category (4) crystallizes in the non-centrosymmetric cubic structure. Previously we studied the split Fermi surfaces properties of $LaCoGe_3$, $LaRhGe_3$, and $LaIrGe_3$ with the Rashba-type tetragonal structure, via the dHvA experiment and energy band calculation [3]. The splitting energy of the main branch α is 460 K in $LaCoGe_3$, 510 K in $LaRhGe_3$, and 1090 K in $LaIrGe_3$. The splitting energy becomes large for a change of Co-3d, Rh-4d, and Ir-5d electrons. The splitting energy is thus expected to become larger for Th-6d electrons of $Th_3Ni_3Sn_4$.

Lastly, we will enjoy with growing various kinds of P and Sn based compounds such as MnP, Mn_2P, Cu_3P, and Sn_4P_3. The technique of the single crystal growth for the P-based compounds is mainly due to the Sn-flux and chemical transport methods. For example, high-quality single crystals of MnP have been recently grown by the Sn-flux method, with the residual resistivity ratio of RRR = 1200.

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Itinerant multipolar order in spin-orbit coupled metals

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Novel quantum phases emerging in the presence of strong spin-orbit coupling (SOC) are recently attracting particular attention in condensed matter physics. The multipolar phase with spontaneously broken inversion symmetry is one of the exotic phases predicted to be realized in correlated metals with SOC [1]. The lack of inversion symmetry lifts spin degeneracy and generates spin-polarized Fermi surfaces in a spin-orbit coupled metal. A promising candidate for hosting the SOC driven multipolar phase is the metallic 5*d* pyrochlore oxide $Cd_2Re_2O_7$. This compound undergoes two structural transitions at $T_{s1} \sim 200$ K, and $T_{s2} \sim 120$ K and the inversion symmetry is lost below T_{s1} [2]. Although the structural change across the transition at T_{s1} is extremely small, resistivity decrease steeply and the magnetic susceptibility shows a remarkable reduction. Therefore, the structural transition at T_{s1} is considered to originate from electronic instability. Recent optical second harmonic generation study has suggested the presence of a multipolar order below T_{s1} [3]. However, experimental evidence for spin-split Fermi surfaces expected for the multipolar order remains missing.

We present a quantum oscillation study of the spin-orbit coupled metal $Cd_2Re_2O_7$, which reveals spin-split Fermi surfaces of this compound for the first time [4]. In the previous studies, it was difficult to detect quantum oscillation owing to the lack of high-quality single crystals. Our continuous effort to improve the sample quality has resulted in obtaining high-quality single crystals with residual resistivity ratio up to 300, which is one order of magnitude higher than those of previously prepared crystals. The high-quality crystals have enabled us to observe de Haas-van Alphen (dHvA) oscillations, clearly as shown in Fig. 1a. The fast Fourier transform spectrum of the dHvA oscillations (Fig. 1b) gives some dHvA frequency branches, which are proportional to the extremal cross-sectional areas of Fermi surfaces. We measured the angular dependence of the dHvA frequencies and observed spin-split electronic Fermi surfaces centered at the Γ point.

$Cd_2Re_2O_7$ provides a unique opportunity to search for novel magnetoelectric effects realized in the multipolar ordered metals.

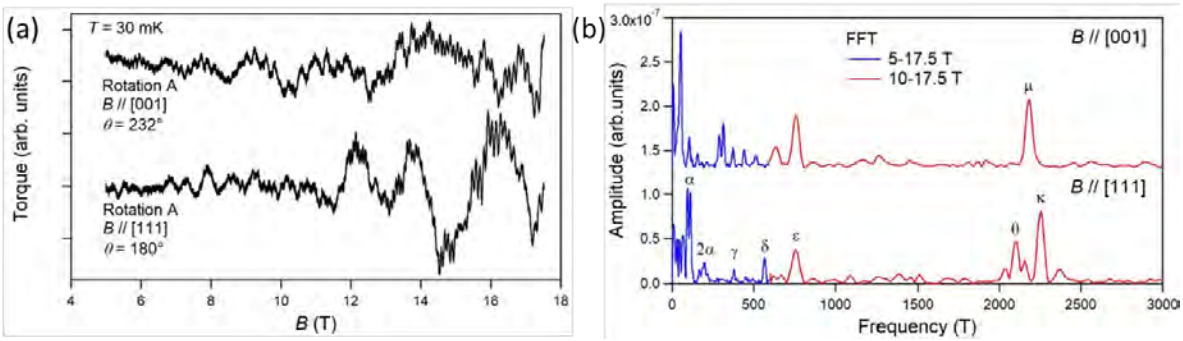

Fig. 1. (a) Field dependence of the magnetic torque at 30 mK with a magnetic field applied along the [001] and [111] directions. (b) Fast Fourier transform spectrum of the de Haas-van Alphen oscillations.

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Odd-parity multipole order and parity-fluctuation superconductivity in $Cd_2Re_2O_7$ under high pressure

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Pyrochlore superconductor $Cd_2Re_2O_7$ shows two structural transitions at ambient pressure. Cubic pyrochlore structure at room temperature (phase I) transforms to the tetragonal structure without inversion symmetry in phases II and III. The transition at T_{s1} has been regarded as a band Jahn-Teller transition due to the band structure with high degeneracy in the high-symmetric pyrochlore structure. As a result, tiny crystal deformation leads to the drastic change in the transport properties. [1] Application of pressure suppresses these transition temperatures and induces many phases (IV-VIII). [2, 3] The inversion symmetry survives in the pressure-induced phases V and VIII above $P_c \sim 4.2$ GPa. The superconducting transition temperature T_c increases with increasing pressure in phase III and reveals no drastic change in phases IV, VII and VIII. On the other hand, the upper critical field B_{c2} strongly increases with increasing pressure. Recently the theoretical scenario was suggested, where the fluctuation of T_{s1} transition generate an attractive pairing interaction in an odd-parity pairing channel, which promotes the odd-parity superconducting state. [4]

In this study, we will investigate the pressure dependence of the superconducting gap with the heat capacity and NMR measurements. We also investigate the electronic state in the pressure-induced phases with the Hall effect measurement and search the parity-fluctuation effect. From these experimental studies, we clarify the characteristic transport properties and superconductivity with the multipole origins in $Cd_2Re_2O_7$.

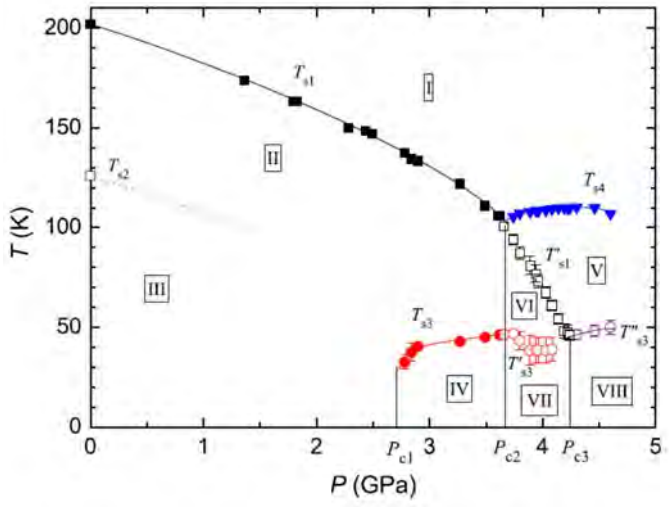

Fig. 1. Pressure-temperature phase diagram of $Cd_2Re_2O_7$. [1]

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Observations of multipole's order and localized-itinerant duality

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In this research project, we investigate 4*f* electronic states in rare-earth compounds in terms of localized-delocalized transition and multipole order. The detailed mechanism of the localized-delocalized transition in rare-earth compounds having a multi-*f* electron configuration have not been clarified. As shown in Fig. 1, we have recently studied the pressure and temperature dependences of Sm valence υ_{Sm} in SmB_6, which is well known as a prototypical intermediate valence compound, by x-ray absorption spectroscopy measurements [1]. The results clearly show that, at the critical pressure P_c of the nonmagnetic-magnetic transition (P_c=7-10 GPa), υ_{Sm} is far below 3, *i.e.* magnetic trivalent state. Moreover we found out that the deviation from 3 is attributed to the two different characteristic components: one is associated with low-energy electronic correlations involving Kondo like behaviour, and the other is associated with high-energy valence fluctuations. Interestingly, the robustness of the strong valence fluctuations at P_c is common to some other Sm compounds as well, but markedly different from already known cases of Ce and Yb compounds. By considering that trivalent and divalent Sm ions possess $4f^5$ and $4f^6$ configuration, respectively, the results suggest that the localized-delocalized transition in the multi 4*f* electron systems can be accompanied with such a dual nature. We are planning to carry out similar systematic measurements on other Sm-based intermediate valence compounds in this project.

We have also succeeded in observing ^{11}B-nuclear quadrupole resonance (NQR) signal of CeB_6 at extremely low frequency and zero magnetic field. CeB_6 shows the antiferroquadrupole (AFQ) order, and the realization of O_{xy}-type AFQ order is suggested mainly from neutron scattering and nuclear magnetic resonance measurements in magnetic field [2,3]. However, its AFQ ordered structure in zero field has not been well identified experimentally, because there is little tool to observe AFQ order without involving field-induced magnetic components, such as magnetic dipoles and octupoles. Since the NQR measurement is an experimental technique to detect changes in local charge distribution through electric field gradient at an observing nuclei position, we expect that the present experiments will bring new information on the AFQ ordered state at zero field.

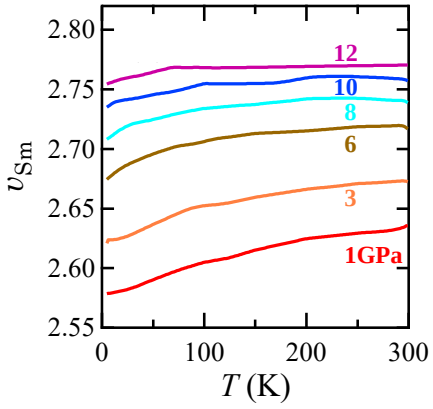

Fig. 1. υ_{Sm} - T curves of SmB_6 at representative constant pressures [1].

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Theoretical study of new quantum phenomena related to valence transition

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Unconventional quantum criticality discovered in heavy-electron quasicrystal (QC) $Yb_{15}Al_{34}Au_{51}$ has attracted great interest [1]. The criticality is common to those observed in periodic crystals β-$YbAlB_4$ [2] and α-$YbAl_{1-x}Fe_xB_4$ (x=0.014) [3], which is well explained by the theory of critical Yb-valence fluctuations (CVF) [4]. The QC $Yb_{15}Al_{34}Au_{51}$ exhibits robust criticality under pressure and a new type of scaling called T/B scaling, which are also explained by the theory of the CVF [5,6]. Recently-measured lattice-constant dependence of the Yb valence in the QC $Yb_{15}(Al, Ga)_{34}(Au, Cu)_{51}$ [7] is naturally understood from the viewpoint that $Yb_{15}Al_{34}Au_{51}$ is located at the quantum critical point (QCP) of the valence transition [8].

Recently, *not* diverging Grüneisen parameter Γ toward the lowest temperature T =70 mK has been observed in the QC $Yb_{15}Al_{34}Au_{51}$ [9]. Surprisingly, its absolute value |Γ| at T =70 mK is smaller than that in the 1/1 approximant crystal (AC) $Yb_{14}Al_{35}Au_{51}$, which shows the Fermi-liquid behavior. This poses a serious challenge to the conventional understanding that |Γ| diverges at *any* QCP [10].

To clarify the mechanism, first we have constructed the complete framework for calculating the specific heat C, the thermal-expansion coefficient α, and the Grüneisen parameter Γ near the magnetic QCP on the basis of the theory of spin fluctuations [11]. We have succeeded in deriving analytical expressions of C, α, and Γ, which consist of not only the critical term but also non-critical term for ferromagnetic and antiferromagnetic (AFM) QCPs in 2- and 3-spatial dimensions. This framework gives thermodynamically-consistent expressions of C, α, and Γ each other, which covers whole temperature region ranging from the low-T critical to high-T Curie-Weiss regimes. We have discovered the existence of the temperature-dependent coefficient in the critical term [11], which has not been reported previously [10]. This affects temperature dependences of α and Γ and even affects the criticality for the 2d AFM case, which is different from the one reported in [10]. It is clarified that the divergence of Γ arises from the inverse susceptibility renormalized by the mode-mode coupling of spin fluctuations coupled to the volume for each class of QCP [11].

This formalism makes it to possible to construct the theory of the specific heat C, the thermal-expansion coefficient α, and the Grüneisen parameter Γ near the QCP of the valence transition in a unified way.

In the presentation, we will overview the current status of the experiment and theory and will discuss the prospect of new quantum phenomena related to the valence transition.

This presentation is based on the work done in collaboration with K. Miyake.

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Charge ordering and heavy fermion due to orbital-dependent hybridization in rare-earth compounds

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Recently, it has been revealed that the low-temperature phenomena of rare-earth systems are often governed by the properties of c-f hybridizations that depend on the symmetry of the 4f orbitals. In this project, we would like to explore the theoretical consquences on the novel charge (and/or multipole) ordering and the heavy fermion states derived from such orbital-dependent hybridizations.

One typical example is $SmRu_4P_{12}$ that shows a fascinating metal-insulator transition associated with an orbital ordering of 4f electrons in Sm ions at finite magnetic fields [1]. In fact, recent theoretical studies show that an extended Kondo-lattice model based on the realistic hybridization can successfully explain the anomalous features of this material [2]. The most prominent characteristic of the model is an interaction between the charge density of conduction electrons and the orbital occupancy of f electrons, which has a universal nature in a class of the hybridizations, not specific to $SmRu_4P_{12}$. Therefore, we have recently studied the phase diagram of the extended Kondo-lattice model at zero magnetic field for general band filling, within the two-sublattice mean-field approximation. Then, it is particularly found that a small amount of hole doping destabilizes the antiferromagnetic insulating phase at half filling and brings alternatively a novel spin-charge composite order phase in a low- and intermediate-doping region. The mechanism of the phase competition is clearly explained in terms of unusual quasi-particle states in the composite order phase. We will study in near future the possibility of stabilizing the composite ordered phase with longer periodicities beyond the two sublattices, in order to construct a more quantitative phase diagram. The studies in this direction must be useful to explore the relationships with complex ordering phenomena observed in other Ce and Sm compounds [3,4].

We also plan to investigate the peculiar properties of the field-insensitive heavy fermion (FIHF) in some Sm compounds such as $SmOs_4Sb_{12}$, $SmTa_2Al_{20}$ and so on [5,6]. Considering that Sm^{2+} has the f^6 spin-orbit coupled ground singlet, we have already introduced a two-orbital impurity Anderson model with an effective f^2 singlet ground state in the localized limit, and have studied the ground-state and Fermi-liquid properties of the model by employing the numerical renormalization method [7]. On this basis, we will study in this project the properties of the Anderson model with more realistic multiplet structures of Sm ions in order to clarify the conditions of forming FIHF in Sm systems. In addition, we will also study the explicit dependences of the properties on the magnetic field.

In analogy with such Sm compounds, we would like to study the Eu compounds as well, in which the f^6 singlet state is again relevant to Eu ions. It is well known that the Eu compounds often display distinct valence transitions at intermediate valences with applying the pressure and/or substituting constituent atoms. We will try to clarify the origin and the condition of the transition, by investigating similarity and dissimilarity with Sm ions in terms of the characteristic multiplet structures.

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Quantum Spin Nematic Phase of Frustrated Systems

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The quantum spin nematic phase, which is a kind of multipole phases, has attracted a lot of interest in the field of the strongly correlated electron systems, as well as the quantum spin liquid phase. Using the numerical exact diagonalization, the density matrix renormalization group (DMRG) calculation, and the finite-size scaling analysis, it is found that some quantum spin nematic and spin liquid phases appear in the anisotropic and/or frustrated quantum spin systems.

In our previous work, quasi-one-dimensional quantum spin systems with the easy-axis anisotropy in magnetic field are theoretically investigated using the numerical exact diagonalization, the density matrix renormalization group (DMRG) and the finite-size scaling analysis[1]. It was found that a field-induced nematic phase appears at some critical field in the anisotropic spin ladder and the mixed spin chain. The nematic phase is characterized by the power-law decay in the correlation function of the second-order spin moment. In addition at some higher critical field a quantum phase transition can occur to the conventional field-induced Tomonaga-Luttinger liquid. Several typical magnetization curves calculated by DMRG are presented. We will also propose an experiment to observe these field-induced transitions by NMR measurements. The field-induced incommensurate order observed in azurite, which is modeled by the distorted diamond chain, by the recent NMR measurement will be also discussed.

Recently the field-induced nematic phase was observed on the frustrated spin ladder system[2,3]. So we study on a frustrated spin ladder system[4], using the numerical diagonalization and DMRG. As a result, it is found that several exotic quantum phases, including the spin-nematic liquid phase. We also report some exact eigenstates of the present model and present several interesting phase diagrams[5].

We also obtained some new results about the magnetization process of frustrated systems; the triangular lattice quantum antiferromagnet with the next-nearest-neighbor interaction[6], or with the lattice distortion[7,8]. Those results will be presented.

As a future plan, we propose the theoretical and computational studies on the carrier doped strongly correlated electron systems in the quantum spin nematic phase. Some exotic transport phenomena induced by the spin nematic order or the two-magnon bound state.

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Development of Strongly Correlated Multipole Materials: Plan and Perspective of D01 Group

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In this research, we will develop novel materials necessary for studying the physics of strongly-correlated multipole-conducting systems with “parity mixing” and “zigzag structure” as keywords, and search for exotic phenomena caused by parity-mixing effects. The zigzag structure stands for structures that have no spatial inversion symmetry at the atomic position and have it at the centre of the bond. Examples of such structures are a one-dimensional zigzag structure, a two-dimensional honeycomb structure, and a three-dimensional diamond structure. When heavy atoms are placed in these structures, it is expected that a novel degree of freedom, namely, a strongly correlated multipole is produced because of the strong parity mixing and spin orbit coupling. We expect that such multipoles are essential for the emergence of novel quantum transport such as exotic superconductivity.

Potential candidates are SrPtAs ($P6_3/mmc$, D_{6h}^4, No. 194) and BaPtSb ($P\bar{6}m2$, D_{3h}^1, No. 187) superconductors with a honeycomb network [1, 2]. For SrPtAs, theoretical studies have predicted a singlet-triplet mixing state [3], a chiral *d*-wave state [4], and an *f*-wave state [5]. mSR measurements suggested a chiral *d*-wave state [6], while NMR/NQR suggested a conventional *s*-wave state [7]. The controversy in experiments will be settled by using single crystalline samples, which we have succeeded to synthesize recently. In addition, spin-split Fermi surfaces will be examined by angle-resolved photoemission spectroscopy and quantum oscillation measurements.

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Exploration of Novel 5*d* Electron Systems "Breaking" Inversion Symmetry

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Inversion symmetry is one of the most important symmetries in solid state physics. In particular, 5*d* electron systems are expected to show exotic electronic phenomena coming from the inversion symmetry breaking, because the strong spin-orbit coupling and electron correlation coexists in them. In this study, we try to find such phenomena by exploring novel 5*d* electron systems, where the inversion symmetry is "broken" by the following two ways.

One is the exploration of 5*d* electron systems that show a temperature- or pressure-induced phase transition accompanied by inversion symmetry breaking. As in the case of a pyrochlore oxide $Cd_2Re_2O_7$ [1,2], the inversion symmetry breaking can be an essential ingredient driving such a phase transition. Furthermore, we can extract the effect of inversion symmetry breaking by comparing the physical properties before and after the phase transition. We plan to find such phase transitions in 5*d* transition metal compounds with pyrochlore and kagome structures.

The other is the 5*d* transition metal compounds with "extended zigzag structure" such as honeycomb and diamond structures, where inversion symmetry is preserved in the whole crystal structure but is locally broken at the atomic sites. The materials with the extended zigzag structure are expected to show significantly different physical properties from those without global inversion symmetry. In particular, the fact that MgB_2, ZrNCl, and LnFeAsO have the extended zigzag structure implies that this structure is favourable for realizing high T_c superconductivity. We will organize the 5*d* transition metal compounds with extended zigzag structure by the crystal symmetry and explore the exotic electronic phenomena in the focused materials.

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Study on Novel Phenomena in Geometrically Frustrated Iridates

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Studies on the physical properties of Ir oxides for the last ten years have revealed the importance of spin-orbit interaction. The purpose of our project to reveal novel phenomena in geometrically frustrated iridates of $Ln_2Ir_2O_7$ and $Ca_5Ir_3O_{12}$.

(I) Pyrochlore iridates $Ln_2Ir_2O_7$ (Fd-3m, No. 227) for Ln=Nd, Sm, Eu, Gd, Tb, Dy, and Ho indicate metal-insulator transition (MIT) at 33, 117, 120, 127, 132, 134, and 141 K, respectively [1]. The MIT involves AFM state with Ir moments with "all-in/all-out" configuration which is considered to be octupole ordering [2]. Theoretical study for pyrochlore iridates predicts a new quantum critical phenomena (QCP) around a disappearance of AFM with "all-in/all-out" configuration by chemical doping [3]. We have investigated the effect of chemical carrier doping for pyrochlore iridates in order to reveal the theoretically predicted QCP and novel quantum phase.

(II) $Ca_5Ir_3O_{12}$ has a hexagonal structure with noncentrosymmetric space group of P-62m (No. 189) [4]. In the crystal structure, it should be noted that one-dimensional chains of the edge-sharing IrO_6 form triangular lattices in the c-plane (Fig. 1). $Ca_5Ir_3O_{12}$ has a mixed valance state of Ir^{4+} and Ir^{5+} and the averaged valence of Ir ions is +4.67. It is reported that $Ca_5Ir_3O_{12}$ shows a semiconducting conductivity and AFM ordering below T_N =7.5 K [4]. In addition, $Ca_5Ir_3O_{12}$ indicates a second order phase transition at 105 K, where the specific heat shows a sharp anomaly and the electrical resistivity shows a sharp bending [4]. The origin of phase transition at 105 K is not clear at present as the structural and magnetic transitions have not been confirmed in XRD, neutron scattering and μSR measurements for the polycrystalline samples [4,5]. Recently, we discovered that $Ca_5Ir_3O_{12}$ along c-axis shows nonlinear conductivity below room temperature by using the pulse sweep method (Fig. 2) [6]. We have investigated the origin of phase transition at 105 K and the nonlinear conductivity by using experimental and theoretical approaches.

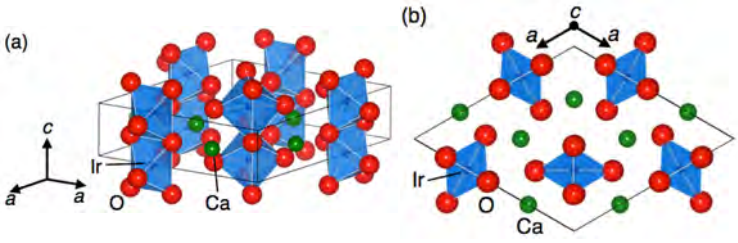

Fig. 1. (a) Crystal structure of $Ca_5Ir_3O_{12}$ [6]. (b) Sublattice of Ir form triangular lattice in the c-plane [6].

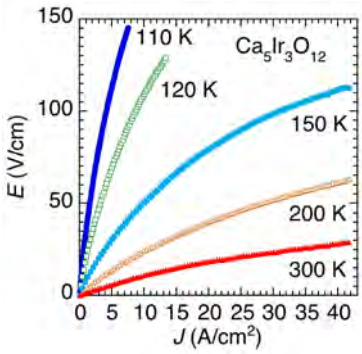

Fig. 2. Current density-electric field (J-E) curves of $Ca_5Ir_3O_{12}$ along c-axis [6].

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Control of anomalous electronic states related with spin-orbit interaction in 2- and 3-dimensional transition metal compounds

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The transition-metal chalcogenides and pnictides show a variety of interesting properties related with electron correlation and spin-orbit interaction. MX_2 and MXPn (M=transition metal, X=S, Se, Te, Pn=P, As, Sb, Bi) are famous chalcogenide and pnictide systems. In this work, we are studying MX_2, MXPn (M=Ni, Pd and Pt) and related systems to explore the new physical properties. These systems have various electronic state coupled with the crystal structures.

First we focus on MTe_2 (M=Ni, Pd and Pt) in this work. Recent experimental studies on $PdTe_2$ and $PtTe_2$ with CdI_2–type layered structure have indicated that these systems have new exotic electronic state, type II Dirac fermion state [1,2]. The results of angle resolved photoemission spectroscopy (ARPES) have revealed that the Dirac point exists at $(0,0,k_z)$ and the Dirac cone is strongly tilted along Γ-A direction (k_z-direction) in $PdTe_2$ and $PtTe_2$.

Our ARPES result for $NiTe_2$ indicates that this compound also has type II Dirac cone. The Dirac point exists very near Fermi level (E_F) in $NiTe_2$, while they in Pd and Pt system are located around -0.5 ~ -0.8 eV below E_F. In this work, we will try to control the energy level of Dirac point by hole or electron doping and search the anomalous magnetotransport properties related with Dirac fermions.

Second target of our study is $PdSe_2$ and related materials. $PdSe_2$ has 2-dimensional $PdSe_2$-type structure, and undergoes the structural phase transition from $PdSe_2$-type to 3-dimensional pyrite structure by applying pressure. Recent study on $PdSe_2$ indicates that this material shows the superconductivity with T_c~13 K in the high-pressure pyrite phase [3]. In our work, we try to control this structural phase transition under the ambient pressure by the chemical doping to $PdSe_2$. $NiSe_2$ and $RhSe_2$ are famous pyrite materials, and the solid solution systems of $Pd_{1-x}Ni_xSe_2$ and $Pd_{1-x}Rh_xSe_2$ with pyrite structure can be synthesized by the high pressure method [4,5]. These doped $PdSe_2$ systems are expected to show the semiconductor to metal transition concomitantly with the structural phase transition. We'll search the superconductivity in the vicinity of the semiconductor-metal transition, and clarify its origin in these solid solution systems.

The pnictogen substitution to $PdSe_2$ is also expected to induce the structural phase transition to pyrite lattice. For example, PdSeBi has a non-centrosymmetric ullmannite structure [6], which is related to the pyrite structure. We try to synthesize the solid solution system $PdSe_{2-x}Pn_x$ using high pressure method, and investigate the critical phenomena in the vicinity of semiconductor-metal transition and structural phase transition.

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Giant negative and positive magnetoresistance in $BaMn_2Pn_2$ (Pn = As, Sb, Bi)

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In this start-up meeting of J-Physics, we report intriguing magnetotransport phenomena observed in $BaMn_2Pn_2$ (BMPn) compounds, where Pn stands for the pnictogen elements (Pn=As, Sb, and Bi). Being well recognized as the (122) layered structure of Fe pnictides of $BaFe_2As_2$ (BFA) discovered recently as a new high Tc superconductor family in the framework of a medium electron-correlated regime, the same stoichiometric combination of the three Pn elements successfully allows the existence of BMPn compounds with the same crystal structure (tetragonal 122-structure with I4) for all Pn elements including P. Intriguingly, not only the crystallographic but also the G-type antiferromagnetic (AF) spin ordering perpendicular to the square Mn-plane is identical in all BMPn's, and this can be compared to the stripe-type AF spin-ordering parallel to the square Fe-plane in BFA. Magnetotransport properties of BFA, being known as a compensated multiband semimetal with tiny Dirac cone states of both electrons and holes [1] in the itinerant regime, generally obey the law of semiclassical transport theory [2], which clearly suggests that the magnetoresistance (MR) should be minimized when magnetic field (B) is aligned parallel to the charge current (j). On the other hand, BMPn compounds have been considered as a local AF insulator in the localization regime, the origin of which can be related to the strong Hund coupling of electron spins residing on Mn^{2+}. Strong hybridization between 3d-Mn and p-Pn orbitals has also been considered to provide significant effects on the electronic structure and the magnetism of BMPn's. Consequently, a BMPn family of materials could be particularly intriguing from the view point of symmetry and electron kinetics. The magnetic point group of BMPn's is 4'/m'mm', whose parity is odd under both time reversal (TR) and space inversion (SI) symmetries, and hence so-called PT symmetry under the combination of TR and SI is preserved. Recently, an intriguing magnetic hexadecapole ground state has been proposed in these materials [3]. Importantly, by changing the Pn element in BMPn, one can tune both spin-orbit coupling (SOC) and p-d hybridization while holding the crystallographic and the magnetic structure unchanged. In this J-Physics research project: Physics of Multipole Conductive System in Grant-in-Aid for Scientific Research on Innovative Areas, we will perform the first systematic observations on the magnetotransport properties of BMPn compounds in a wide range of magnetic field (B) and temperature (T). All three compounds show very large positive and negative magnetoresistance (MR) with unique and complex dependences both on B and T. The observed MR shows a geometrically special anisotropic symmetry under B that cannot be understood by any theoretical models available so far. When Pn elements were changed from As to Bi, the observed MR importantly shows a systematic variation in both its magnitude and B-dependence. In the extreme B regime, the MR of BMBi becomes the largest towards a metal in the smallest B-range among the BMPn's.

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Ordered States in Two Channel Anderson Lattice Model.

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Non-Fermi liquid behaviors in the resistivity have been reported in PrV_2Al_{20} [1] and $PrIr_2Zn_{20}$ [2]. Namely, the electrical resistivity is in proportion to $T^{0.5}$ in rather wide low T region above the quadrupolar transition temperature T_Q. The Specific heat increases like $C_0-C_1T^{0.5}$ as T decreases at $T>T_Q$. The ground state of the crystalline-electric field (CEF) of the local f-electron was identified to be the Γ_3 non-Kramers doublet in $4f^2$ configuration [2]. Such a system in f^2 configuration is expected to exhibit an anomalous behaviors associated with the two-channel Kondo effect.

Tsuruta *et al.* investigated electronic states in the M-channel Anderson lattice model using the expansion from the limit of large spin-orbital degeneracy N ($1/N$-expansion) [3], and showed that the inclusion of the self-energy of $O((1/N)^0)$ leads to heavy electrons with degeneracy of channel and spin-orbit. In the single channel case, the imaginary part of the self-energy of conduction electrons (ISE) exhibits the Fermi liquid behavior: i.e. ISE is given by a form proportional to T^2 owing to the inter-site correlation effects in higher order terms in power of $1/N$.

In the two-channel case, however, a T-linear term in ISE at the Fermi level, in contrast to a T^2-term in the Fermi liquid is found in the limit of $T \to 0$. However, a $T^{0.5}$ dependence appears in a rather wide low T region, which explains quite well the non-Fermi liquid behavior observed experimentally.

Because of the anomalous T dependence of ISE, the chemical potential is given by $\mu_0-\mu_1T^{0.5}$, and the specific heat is given by $C_0-C_1T^{0.5}$. We also obtain the scaling behavior $f(T/T_0)$, T_0 is defined as the crossover temperature at which the T dependence of ISE starts to deviate from the $\sqrt{T}$ dependence to that with a much lower exponent as T increases, in electrical resistivity, chemical potential, specific heat and magnetic susceptibility, explaining non-Fermi liquid properties observed in Pr 1-2-20 compounds.[4]

We will present the results of the theoretical study of the antiferro quadrupole and superconducting ordered state in Pr 1-2-20 systems.

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Vortex charging effect in s-wave superconductors

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The vortex-core charging in type-II superconductors has been pointed out to be related to the sign change of the flux-flow Hall conductivity, and numerous studies on the charging of a superconducting vortex have been carried out. However, the forces responsible for the charging of a superconducting vortex are not fully understood. This is because all the force terms used to describe charging in superconductors are missing from the standard Eilenberger equations (i.e., the quasiclassical equations of superconductivity) used to study superconductors in a magnetic field microscopically. Although there have been several numerical calculations of the vortex-core charging in superconductors based on the Bogoliubov-de Gennes (BdG) equations, these equations are not suitable for studying the charging mechanism.

We derived augmented Eilenberger equations that incorporate the following missing force terms: (i) the Lorentz force, (ii) the pair-potential gradient (PPG) force, and (iii) the pressure difference arising from the slope in the density of states (DOS) [1]. Recently, augmented Eilenberger equations with the Lorentz and PPG forces have been derived microscopically by studying the Hall and charging effects in superconductors [2, 3], but the pressure due to the slope in the DOS has not yet been considered in augmented Eilenberger equations, despite phenomenological indications that it is a charging mechanism in a vortex of type-II superconductors [4]. This newly added pressure is called "the SDOS pressure". We calculated the charging in an isolated vortex of an s-wave superconductor with a spherical Fermi surface using the augmented Eilenberger equations incorporating the Lorentz force, PPG force, and SDOS pressure. When we compare the charge densities due to the three force terms in the augmented Eilenberger equations, the vortex-core charging due to the SDOS pressure is larger than that due to the other forces near the superconducting transition temperature.

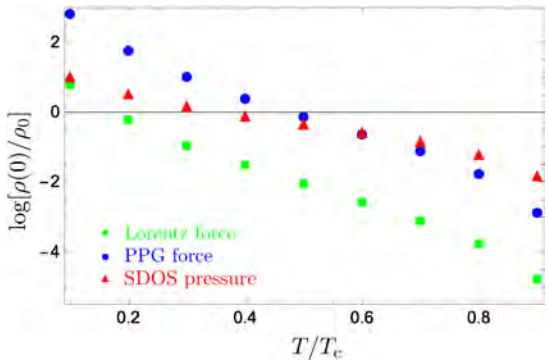

Fig. 1. (Color online) Normalized charge density due to the Lorentz force (green square points), PPG force (blue circular points), and SDOS pressure (red triangular points) at the vortex center as a function of temperature.

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Group-theoretical classification of multipole order

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In these decades, multipole degrees of freedom have attracted a lot of attention in the field of strongly-correlated electron systems. The entanglement of spin and orbital gives rise to exotic quantum phenomena such as novel types of superconductivity and Kondo effect [1]. Recently, there is a growing interest in the multipole order with the parity violation, namely, odd-parity multipole order, while the previous studies focused on the even-parity multipole order. In the odd-parity multipole order, the crystalline sublattice degree of freedom plays an important role, which leads to the intriguing itinerant properties such as spin-momentum locking and anti-symmetric distortions [2]. Therefore, the odd-parity multipole order generates a renewed interest in the multipole physics.

In the presentation, we present the group-theoretical classification of even-/odd-parity multipole order. Following the classification of unconventional superconductivity by Sigrist and Ueda [3], we classified multipole moments by the irreducible representations of a given point group and clarified that the peculiar itinerant properties distortions are associated with the odd-parity multipole order. Furthermore, we investigated emergent responses induced by odd-parity multipole order such as magnetoelectric effect, Edelstein effect, magnetopiezoelectric effect, and dichromatic electron transport in the framework of our classification. We also classified magnetic compounds with the representation analysis and identified a lot of candidates for odd-parity magnetic multipole order. Combining our classification with the list of candidate materials, we predicted the emergent responses of odd-parity multipole materials.

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Electronic structures suitable for the orbital Kondo effect

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The orbital Kondo effect in the *f*-electron system without Kramers degeneracy is an interest research subject in the long term. However, there are little studies focused on the relationship between its origin and the electronic structure. In this work, firstly, we clarify necessary conditions of the occurrence about the orbital Kondo effect with the simplified model. As shown in Fig 1(left), we consider the band model in which the degeneration at Γ point and two conduction bands across Fermi level. Also at Γ point, the band structure has Γ_3 symmetry. Considering freedom of the spin, Γ_3 splits two states, $\Gamma_3 \times \Gamma_{1/2} = \Gamma_7 + \Gamma_8$. In this time, *c-f* hybridization determines the condition of the Orbital Kondo effect. We propose candidates which we can observe orbital Kondo effect using the Density of States(DOS) and *c-f* hybridization from results of ab-initio calculation.

In this study, we report to focus on the result of $PrPb_3$ and $PrMg_3$. At first, we perform the DFT(Density Functional Theory) calculation about $PrPb_3$ and $LaPb_3$ using FLAPW method. In $PrPb_3$, the band structure near Fermi level constituted the hybridized Pr-*4f* and Pb-*6p* electrons(Fig.1(middle)). In $LaPb_3$, the conduction band has Γ_8^+ symmetry at about 0.1Ry. above the Fermi level. Secondly, we calculate the Maximum localized Wannier Functions(MLWFs), and project the tight-binding model and estimate Slate-Koster parameter to estimate the hybridization. Similar case, we calculate about $PrMg_3$. In our calculation and analysis, we concluded that PrPb3 has more suitable electronic structure of orbital Kondo system compare with $PrMg_3$. We discuss the difference of the electronics structure of $PrPb_3$ and that of $PrPb_3$ from point of view about the symmetry of eigenstates, in other word, the irreducible representation of eigenstates.

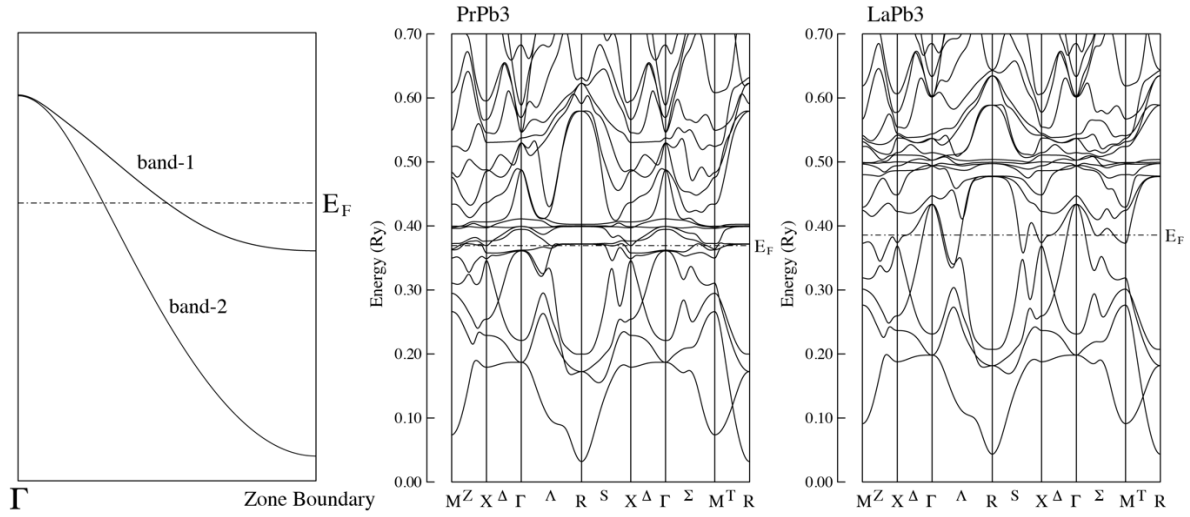

Fig. 1(left). Two degenerated conduction band at Γ point. (middle) electronic structure of $PrPb_3$ (right) electronic structure of $LaPb_3$

Cluster multipole theory for large magneto-optical Kerr effect in antiferromagnets

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Recently, it has been found that Mn_3Sn and Mn_3Ge exhibit a large anomalous Hall effect (AHE) [1,2,3], anomalous Nernst effect (ANE) [4,5] and magneto-optical Kerr effect (MOKE) [6]. In Ref. [7], we introduced a quantity which we call "cluster multipole", and found that macroscopic "octupolarization" is the origin of these anomalous transverse transport phenomena [5].

While there are few antiferromagnetic metals showing a large AHE and ANE, there are many antiferromagnetic insulators for which the Kerr rotation angle is extremely large. In this poster presentation, we are going to show that "octupolarization" is the main origin of the large MOKE in such antiferromagnets [8].

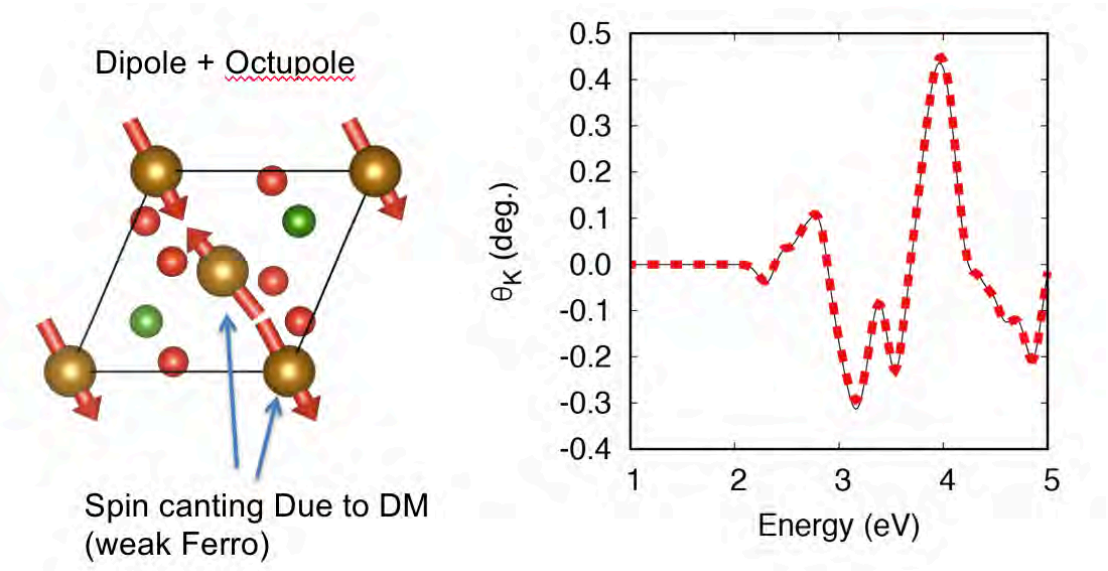

Fig. 1. Magnetic structure and Kerr rotation angle (θ_K) of $FeBO_3$. We see that the contribution of the macroscopic octupolarization (dotted line) is dominant in θ_K.

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Change of Fermi surfaces and multipolar response at transition between crystalline-electric-field- and Kondo-singlets

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In several heavy fermion materials, the crystalline-electric-field (CEF) ground state on each lanthanide- and actinide-ion has f^2-configuration and more intriguing physical phenomena emerge than in f^1-systems. UBe_{13} is a typical example of such compounds and shows non-Fermi-liquid (NFL) behavior and unconventional superconductivity [1]. Since Cox's proposal [2], the quadrupolar Kondo effect with non-Kramers CEF doublet ground state having Γ_3-symmetry has long been believed to be a promising origin of the NFL behavior in UBe_{13}. Recent experiments for $Th_{1-x}U_xBe_{13}$, however, imply that the Γ_1-singlet state is another promising candidate of CEF ground state and the NFL behavior is due to the competition between CEF- and Kondo-singlets [3,4].

Although the impurity Kondo problem with f^2-singlet CEF ground state has been theoretically explored by many authors [5,6], there are few studies on its lattice version [7,8]. In the present study, we investigate the competition between CEF- and Kondo-singlets in the multi-orbital periodic Anderson model on the simple cubic lattice, where we take into account f-orbitals with total angular momentum j=5/2 and conduction d-orbitals with t_{2g}-symmetry. The effects of Coulomb interaction are treated within the rotationally invariant slave-boson mean-field approximation (SBMFA) [9].

Figures 1(a) and (b) show the c-f hybridization (V_{cf})-dependence of the quasi-particle occupation and effective f-level. For V_{cf}<0.56, the CEF-singlet state is realized, while for V_{cf}>0.57, the Kondo-singlet state is realized. Within the SBMFA, the change between CEF- and Kondo-singlet states is 1st-order transition, consistently with the previous study based on a more simplified model [8]. As shown in Figs. 1(c) and (d), across the transition point, Fermi surfaces (FSs) drastically change since in the Kondo-singlet state, f-electrons participate to form the FSs, while in the CEF-singlet state, they do not. It should be noted that the transition is not accompanied by any symmetry breaking and both singlet states are paramagnetic. The f-electron part of multipolar susceptibility $\chi(\boldsymbol{q})$ also shows distinct behavior in each singlet-phase. In the Kondo-singlet phase, $\chi(\boldsymbol{q})$ has moderate $\boldsymbol{q}$-dependence originating from the particle-hole excitation near the Fermi level. On the other hand, in the CEF-singlet state, $\chi(\boldsymbol{q})$ is almost flat in $\boldsymbol{q}$-space since there are only Van Vleck-type contributions to $\chi(\boldsymbol{q})$.

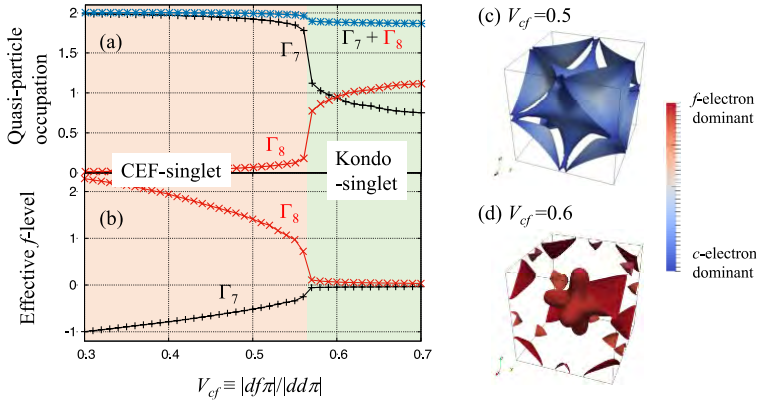

Fig. 1. V_{cf}-dependence of (a) quasi-particle occupation and (b) effective f-level measured from the Fermi level. (c) and (d) Fermi surfaces for CEF- and Kondo-singlet states, respectively.

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Unconventional superconducting gap structure protected by space group symmetry

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Classification of a superconducting gap is one of the central subjects in the research field of unconventional superconductivity. Momentum dependence of the superconducting gap is closely related to symmetry of the superconductivity and the pairing mechanism. Since the superconducting gap structure can be identified by various experiments, combined studies of superconducting gap by theory and experiment may clarify the characteristics of superconductivity. Most of the theoretical studies have been based on the classification of order parameter by the crystal point group, which is summarized by Sigrist and Ueda (called Sigrist-Ueda method) [1]. However, their classification may not provide an exact classification of the superconducting gap.

For example, several studies have shown that the space group symmetry ensures the unconventional gap structures beyond the results of the Sigrist-Ueda method [2-5]. These theories classify not the order parameter, but the superconducting gap itself. Therefore, rigorous results are obtained for gap structures. Regarding point nodes, furthermore, many studies have discussed Weyl nodes in superconductors, namely point nodes protected by a nontrivial topological number [6-8]. However, there are only a few and less-known results about point nodes connected with crystal symmetry [2, 3].

In this study, we classify unconventional line nodes and point nodes beyond the results of the Sigrist-Ueda method using the group-theoretical analysis of the superconducting gap. First, we review the results of symmetry-protected line nodes, clarifying the condition for the existence of line nodes protected by nonsymmorphic symmetry. Next we show our original and useful results; nonsymmorphic-symmetry-protected line nodes appear only on the Brillouin zone face of a primitive or orthorhombic base-centered Bravais lattice. We classify all space groups under the additional constraint. Second, we consider the gap structures on high-symmetry n-fold (n = 2, 3, 4, and 6) axes in the Brillouin zone, as examples of the symmetry-protected point nodes. Surprisingly, the analysis shows the existence of point nodes depending on the Bloch-state angular momentum j_z on a 3- or 6-fold axis. Furthermore, we suggest that such "j_z-dependent point nodes" are realized in a heavy fermion superconductor UPt_3. We also discuss superconducting gap structures in UBe_{13}, SrPtAs, etc.

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Odd-parity multipole fluctuation and superconductivity in non-symmorphic crystalline

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Recent intensive research has clarified novel phenomena of a spin-orbit coupling in locally noncentrosymmetric (NCS) system. For instance, the mixing of spin-singlet and spin-triplet superconductivity [1], odd-parity superconductivity of a pair density state [2], and odd-parity multipole order [3-5]. Motivated by this recent progress, we study an exotic superconductivity induced by *an odd-parity magnetic fluctuation in the vicinity of inversion symmetry breaking*.

The even-parity multipole order commonly appears in the strongly correlated electron system, and many theoretical studies focused on the even-parity multipole order. On the other hand, it has been shown that the odd-parity multipole order is realized in locally NCS crystal [3-5]. More recently, Kozii and Fu [6] have shown that the odd-parity structural fluctuation in the spin-orbit coupled system gives rise to the attractive effective pairing interaction in the odd-parity pairing. Thus, the odd-parity magnetic fluctuation may promote an unconventional pairing.

We investigate a two-sublattice Hubbard model with the sublattice-dependent antisymmetric spin-orbit coupling and Coulomb interaction on the basis of the random phase approximation. We assume a nonsymmorphic and locally NCS structure; the crystallographic point group is D_{4h} and the local point group symmetry at specific ions is D_{2d}, lacking the $\sigma_{v/d}$ mirror reflection symmetry, such as $BaMn_2As_2$ and Sr_2IrO_4.

We find that a magnetic quadrupole, hexadecapole, and toroidal fluctuations appear by the antisymmetric spin-orbit coupling. The B_{2g} (d_{xy}+p-wave) state induced by these fluctuations is more suppressed by a modulate local parity violation than a global inversion symmetry breaking. Our obtained gap function has a gapped/nodal structure protected by the nonsymmorphic symmetry in an inter-sublattice pairing. Furthermore, we obtain two triplet superconductivities, B_{1u} (p+s-wave) and A_{1u} (p+d_{xy}-wave) states. The local parity violation prefers to these triplet states, in striking contrast to the global inversion symmetry breaking.

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Current rectification in $Cd_2Re_2O_7$

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Various multipole ordered states have been intensively studied because of their unique properties, such as non-Fermi liquid and unconventional superconductivity mediated by the electric quadrupole ordering. However, previous studies are limited in the even-parity multipoles because of the presence of spatial inversion symmetry. On the other hand, when the crystal structure breaks spatial inversion symmetry, the odd-parity multipole ordering (magnetic quadrupole and electric octupole, etc…) can be emerged, and various new types of responses to the magnetic and/or electric fields are predicted [1].

Here, we will report the current rectification effect in the metallic $Cd_2Re_2O_7$. $Cd_2Re_2O_7$ is recognized as a candidate of odd-parity multipole ordering at ~200 K by both theory and experiment in recent years [2, 3]. Furthermore, this material also has other interesting properties, such as two characteristic structural transitions and superconductivity in the noncentrosymmetric crystal structure [4]. In the present study, we have clearly observed 2nd harmonic voltage with an ac current excitation under the magnetic field, indicating the presence of current rectification in $Cd_2Re_2O_7$. We found that the magnetic field dependence of current-non-linear signal increases more rapidly than the linear function. This behavior is totally different from the previously reported current rectification in a polar semiconductor, where the Zeeman shift of spin-split Fermi surfaces plays an essential role and the magnetic field response follows a linear function [5]. The magnetic field angular dependence will be also presented.

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Magnetization measurement of $Ce(Ru_{1-x}Rh_x)_2Al_{10}$ ($x < 0.05$) under Electric Current

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Toroidal moment ***t*** is one of the parameters that describe strength of the magnetoelectric coupling. According to a theoretical prediction by S. Hayami *et al*., the toroidal moment can be active even in metallic systems, where the occurrence of exotic phenomena, such as magnetization induced by electric current, is expected [1]. Recently, we experimentally found the electric current-induced magnetization in an antiferromagnetic (AFM) ordered state of a metallic system UNi_4B [2]. However, the observed magnetoelectric effects in UNi_4B cannot be explained in part by the theoretical model. Further investigation in other metallic systems with the toroidal moment are required for full understanding of the magnetoelectric effect.

We now focus our attention on another AFM metallic system $CeRu_2Al_{10}$ and its Rh-doped system $Ce(Ru_{0.95}Rh_{0.05})_2Al_{10}$. They crystallize into $YbFe_2Al_{10}$-type orthorhombic structure with *Cmcm* (D_{2h}^{17}, No. 63), where Ce ions align along *c*-axis forming zigzag structure, with no local inversion symmetry. Magnetic moments of the Ce ions order antiferromagnetically pointing to the *c*-axis at T_N = 27 K for $CeRu_2Al_{10}$, while the magnetic moments of $Ce(Ru_{0.95}Rh_{0.05})_2Al_{10}$ point to the *a*-axis with the AFM ordering below T_N = 24 K [3,4]. Both AFM orders have same propagation vector of $\boldsymbol{q}$ = (0, 1, 0). In the present study, dc *M* measurements under electric current for each setting of $\boldsymbol{I} \parallel a$ and *c*, and $\boldsymbol{B} \parallel a$, *b*, and *c* have been performed using large single crystalline samples provided by H. Tanida. Figure 1 shows the temperature dependence of *M* under $\boldsymbol{I}$ for $CeRu_2Al_{10}$. It is found that the additional *M* (ΔM) is induced by applying electric current below T_N for the three settings: ($\boldsymbol{I}$, $\boldsymbol{B}$) $\parallel$ (*a*, *c*), (*c*, *a*), and (*c*, *b*). Similar ΔM are also observed in $Ce(Ru_{0.95}Rh_{0.05})_2Al_{10}$. We are going to discuss about the cause of the observed magnetoelectric effects in these compounds based on the concept of odd-parity multipoles.

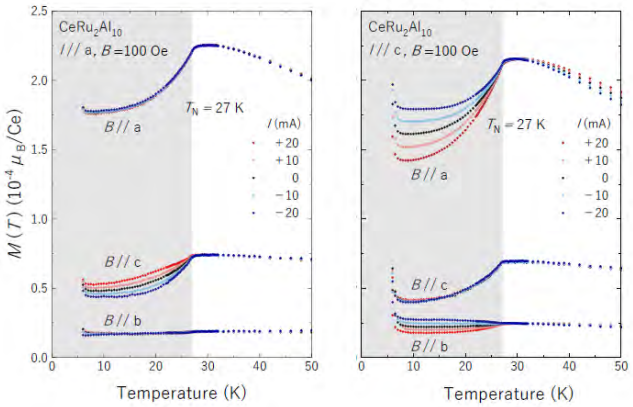

Fig. 1. Temperature dependence of *M* under electric current at $\boldsymbol{B}$ = 100 Oe for $CeRu_2Al_{10}$. (left) $\boldsymbol{I} \parallel a$, and $\boldsymbol{B} \parallel a$, *b*, and *c*; (right) $\boldsymbol{I} \parallel c$, and $\boldsymbol{B} \parallel a$, *b*, and *c*.

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Pulsed high-field NMR study on $CeIn_3$: high-field phase diagram near an antiferromagnetic QCP

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Antiferromagnetic $CeIn_3$ with cubic crystal structure and T_N= 10 K is one of the simplest and best-studied heavy-fermion compounds. In this material, a pressure-induced quantum critical point (QCP) occurs at 2.6 GPa, around which a small dome of superconductivity is observed [1]. The magnetic order can also be suppressed by magnetic field giving rise to a field-tuned QCP at H=61 T [2].

An additional field-induced anomaly was observed in $CeIn_3$ at about 45 T, well inside the antiferromagnetic phase, in tunnel diode oscillator (TDO) measurements [3]. The exact origin of this transition, or crossover, is at present unknown. Remarkably, small heavy *f*-hole pockets of the Fermi surface observed at low magnetic field disappear at about the same field, where an anomaly was observed in the TDO measurements [4]. These small pockets are not predicted by the band structure calculations and are likely to originate from the fragmentation of the large Fermi surfaces that exceed the size the antiferromagnetic Brillouin zone. A similar anomaly in TDO measurements was recently observed at about the same field in $CePt_2In_7$, where a similar change of the Fermi surfaces was also observed [5]. A possible simple explanation of the observations in both $CeIn_3$ and $CePt_2In_7$ is a field-induced change of the magnetic structure from commensurate to incommensurate, which occurs at 45 T. Another, more exciting possibility, is that the 45 T anomaly corresponds to a field-induced transition to a density wave state, as was recently proposed for $CeRhIn_5$ [6].

In order to understand the origin of the field-induced anomaly observed at about 45 T, well before the antiferromagnetic critical field, we have performed a pulsed magnetic field In-NMR study using a single crystal up to 56 Tesla. We confirmed that there is no obvious change of hyperfine fields at In sites even above 45 T. This indicates that there is no structural change at high fields, and further, denies simple explanations of the anomaly as due to a field-induced change of the magnetic structure in $CeIn_3$.

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Linear Dichroism in core level photoemission spectra of cubic PrB_6 on the incommensurate antiferromagnetically ordered phase

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Rare-earth-based strongly correlated electron systems show various interesting phenomena such as competition between magnetism and unconventional superconductivity, charge and/or multipole ordering, and the formation of a narrow (~meV) gap at low temperatures. For clarifying origins of the phenomena, it is important to determine the crystalline electric field (CEF) 4*f* ground-state symmetry.

PrB_6 undergoes an incommensurate and commensurate antiferromagnetically (AFM) ordering at T_N = 7 K and T_{IC} = 4.2 K, respectively [1]. Inelastic neutron scattering measurements have proposed that the Pr^{3+} CEF 4*f* ground-state of PrB_6 is in Γ_5 symmetry [2]. Actually, we have successfully observed the 4*f* ground-state symmetry of PrB_6 in paramagnetic phase by linearly polarized hard X-ray photoemission spectroscopy (HAXPES) [3]. Linearly polarized HAXPES is a powerful method for revealing 4*f* orbital symmetries of strongly correlated electron systems [4,5].

In the present work, we have applied linearly polarized HAXPES to PrB_6 in incommensurate AFM phase, in order to observe the 4*f* electronic structures in incommensurate AFM phase. We have observed the linear dichroism (LD) in HAXPES at BL19LXU of SPring-8. LD is defined as the difference in the spectral weight between the s- and p-polarization configurations. Figure 1 shows the polarization-dependent Pr^{3+} $3d_{5/2}$ HAXPES spectra and LDs in the [100] direction of PrB_6 at 30 K (paramagnetic phase) and 5 K (incommensurate AFM phase). The observed LD and spectra at 30 K are quantitatively reproduced by the simulations for the Γ_5 ground state. On the other hand, the experimental LD at 5 K is slightly suppressed at a binding energy of ~934 eV compared with that at 30 K, which suggests that the LD-HAXPES reflects the electronic structures of AFM-ordered state.

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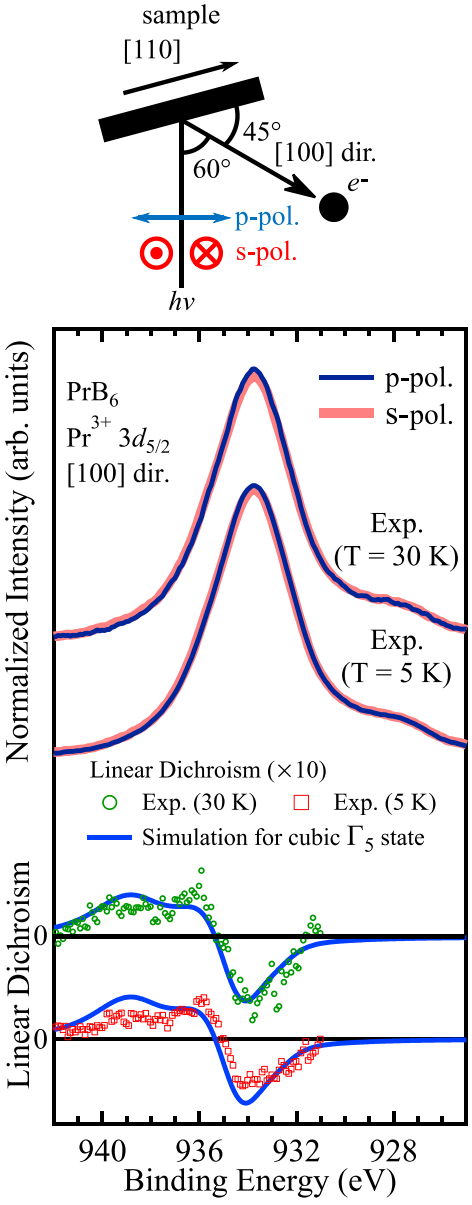

Fig. 1. Polarization-dependent Pr^{3+} $3d_{5/2}$ core-level HAXPES spectra and LDs of PrB_6 at 30 K and 5 K. Experimental LDs are compared with the simulated LD for cubic Γ_5 states along the [100] direction.

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Ground-state 4*f* symmetry in $CeCu_2Ge_2$ probed by soft x-ray absorption and hard x-ray photoemission spectroscopy

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The tetragonal $CeCu_2Ge_2$ shows an antiferromagnetic long-range order below Néel temperature of 4.15 K at ambient pressure [1]. The Sommerfeld coefficient γ is as high as 100 mJ/(mol K^2), suggesting that the energy scale of the on-site Kondo fluctuation is the same order of magnitude as that of the RKKY interaction. External pressure above 7.6 GPa induces superconductivity below 0.6 K due largely to an increase of the hybridization between the localized 4*f* and conduction electrons. Moreover, a different type of superconducting phase emerges at around 12 GPa, where an abrupt change into the critical 4*f* valence fluctuation in the presence of a strong on-site Coulomb repulsion has been proposed to understand its origin [2]. Since the low temperature properties of these compounds are mostly determined by the 4*f* ground state symmetry for Ce^{3+} ions in the tetragonal crystalline electric field, we have performed soft x-ray absorption (XAS) and hard x-ray photoemission spectroscopy on $CeCu_2Ge_2$.

Figure 1 shows the circularly polarized Ce $M_{4,5}$ XAS spectra of $CeCu_2Ge_2$ (top) measured at 6 K. The spectral line shape shows the difference for photon incidence angles of θ = 0 and 54.7° relative to the *c*-axis, especially for the two multiplet peaks at the Ce M_5 edge. This is due to the anisotropy of the spatial distribution of the 4*f* wave function [3]. By using the simulation of XAS spectra based on the Ce^{3+} ionic model, we have revealed the Γ_7 ground-state symmetry of $|\Gamma_7\rangle=\alpha|J_z=\pm5/2\rangle\pm(1-\alpha^2)^{1/2}|\mp3/2\rangle$ with anisotropy factor α^2 = 0.45, reflecting the out-of-plane (parallel to the crystal c-axis) anisotropy in the spatial distribution of the 4*f* states. In the presentation, we will discuss the in-plane symmetry determined by the polarization dependence of the Ce 3*d* core-level hard x-ray photoemission spectra.

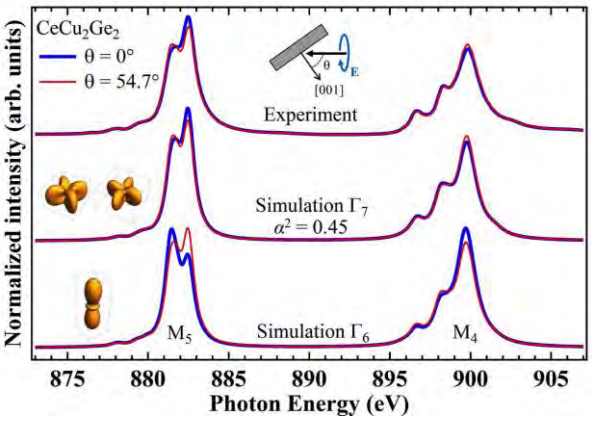

Fig. 1. Circularly polarized XAS spectra of $CeCu_2Ge_2$ at the Ce $M_{4,5}$ absorption edges (top) obtained for x-ray incidence angles of θ = 0 and 54.7° with respect to the c-axis parallel to the surface normal. The spectral simulations assuming the ground state of Γ_7 (α^2 = 0.45), and Γ_6 symmetry together with the initial-state 4f charge distributions.

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Superconducting properties and upper critical field study of $CeIr_3$ single crystal

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The exploration of superconducting properties in Ce-based systems has been one of the most intriguing subjects in the research field of unconventional superconductivity[1]. In this study, we aim to elucidate superconducting properties of $CeIr_3$, which crystallizes in the $PuNi_3$-type rhombohedral structure with the space group R-3m (#166, D_{3d}^5). There are two crystallographically non-equivalent Ce sites (Ce1 and Ce2) and three Ir sites, as shown in Fig. 1. The superconductivity with a transition temperature of 3.34 K in $CeIr_3$ was first reported by Geballe *et al.* in the 1960s[2]. Previous studies were performed at zero field using polycrystalline samples, and the thermodynamic bulk properties have not been reported so far.

Single crystals of $CeIr_3$ were grown by the Czochralski method in a tetra arc furnace under an argon atmosphere. $CeIr_3$ has been reported to be an incongruent melting compounds. We tried the Czochralski method using starting materials with an off-stoichiometric ratio and succeeded in growing single crystals. We obtained single crystals with dimensions of approximately $1.5 \times 1.0 \times 1.0\ mm^3$, as shown in the inset of Fig. 2. The superconducting properties of $CeIr_3$ single crystal are investigated by electrical resistivity, specific heat, and magnetization. Figure 2 shows the temperature dependence of specific heat in the form of C/T and exhibits a clear jump corresponding to the superconducting transition at 3 K, indicating bulk superconductivity in $CeIr_3$. We will discuss the superconducting properties and temperature dependence of upper critical field of $CeIr_3$ single crystal in the presentation.

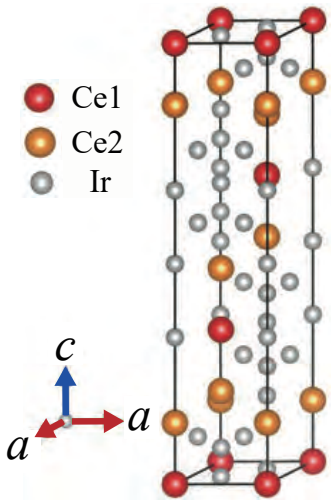

Fig. 1. Rhombohedral crystal structure of $CeIr_3$.

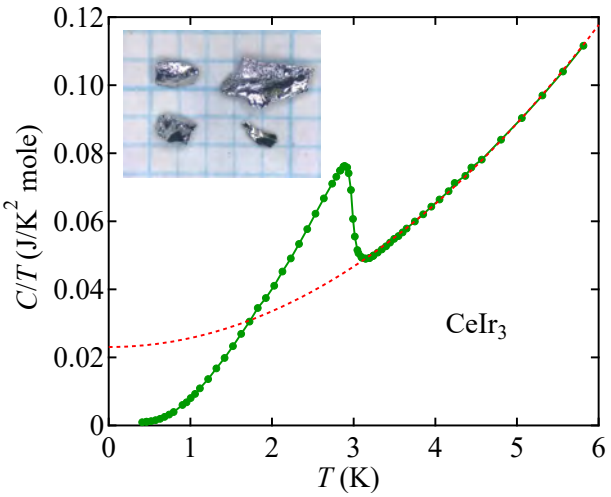

Fig. 2. Temperature dependence of the electronic specific heat of $CeIr_3$ single crystal. The inset shows pictures of $CeIr_3$ single crystal.

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Analysis of electronic states of the rare-earth hexaborides based on the effective Wannier models

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Electronic states of the rare-earth hexaborides RB_6 (R=La,Ce,…,Lu) have been one of the central issues in the heavy Fermion systems and extensively studied theoretically and experimentally for understanding of the *f* electron nature [1]. For example, CeB_6 is a typical and remarkable material exhibiting a rich phase diagram [2] of the magnetic and electric multipole orders, regardless of its simplest $4f^1$ state in Γ_8 quartet crystalline electric field (CEF) ground state. In general, whether the *f* electron behaves itinerant or localize is important and is naively determined by the Kondo temperature T_K vs the ordering temperature T_{RKKY} of the Ruderman–Kittel–Kasuya–Yosida (RKKY) mechanism. In most RB_6 compounds, the 4*f* electron is localized ($T_K<T_{RKKY}$), and their Fermi surfaces are almost similar to that of LaB_6 confirmed by the recent photoemission tomography and high-resolution angle resolved photoemission spectroscopy (ARPES) [3]. In such the localized picture, the multipole orders should be described by the RKKY interaction [4] and their ordering wavevector $\boldsymbol{Q}$ can be determined by the $\boldsymbol{q}$-dependence of the conduction electron susceptibility. Therefore, the microscopic description of the conduction electron state by the realistic Wannier orbitals is important for clarifying the origin of the multipole order [4]. In this study, we analyse the electronic states of RB_6 based on the first-principles band calculation and their effective Wannier models.

First we calculate electronic states of RB_6 (R=La-Lu) by using the WIEN2k package, and construct the two effective Wannier models for LaB_6 by the method of the maximally localized Wannier models [5]. Figure 1 (a) and (b) show the 37 orbital (La-*fds*,B-*ps*) model and the 30 orbital (La-*ds*,B-*ps*) model together with the bandstructure by WIEN2k, respectively. In Fig. 1 (b), the 4*f* level is shifted by GGA+*U* method so as to eliminate the 4*f* contribution in the conduction band. The conduction electron susceptibility and the detail of the RKKY interactions are discussed in the day of the presentation.

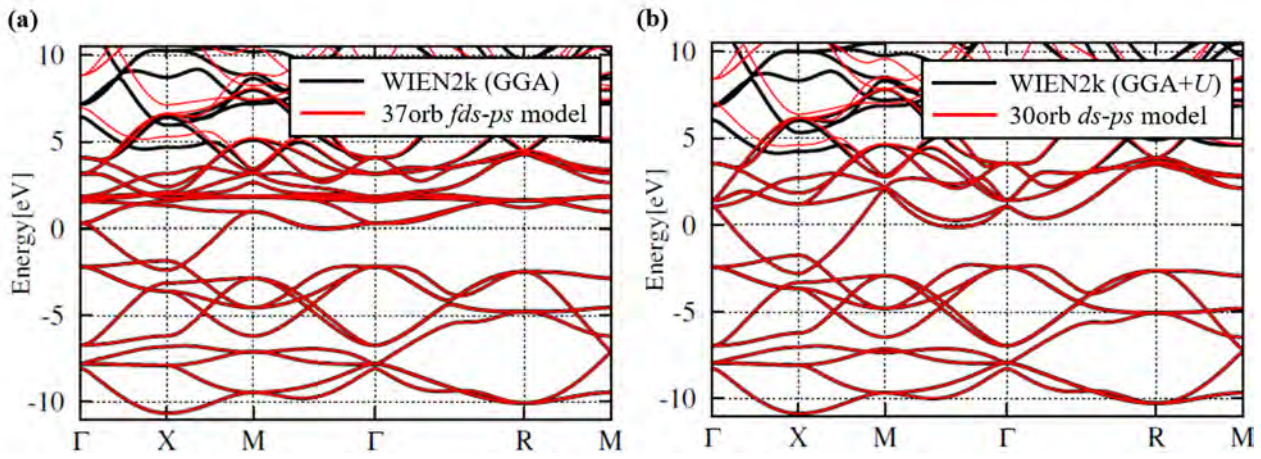

Fig. 1. (a) Bandstructure of LaB_6 by WIEN2k (black line) and the effective Wannier models (red line) with 37 orbital La-*fds* and B-*ps*. (b) Bandstructure of LaB_6 by WIEN2k with the GGA+*U* method for La-4*f* level (black line) and the effective Wannier models (red line) with 30 orbital La-*ds* and B-*ps*.

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Ultrasonic measurements on the possible topological system HoSb

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Investigations on the rare-earth monopnictides (REM) can be traced back more than half a century. The recent discovery of topological properties in REM sparked again intense research activity on the determination of bulk and surface states. Different from topological insulators where the topological surface states form Dirac fermions in the bulk gap, REM belongs to topological semimetals which possess three-dimensional Dirac or Weyle fermions with linear dispersions as bulk states. [1]

The REM, which are described by the formula RX_p (R = rare-earth, X_p = N, P, As, and Sb) exhibit a wide variety of interesting quantum phenomena as changing R or X_p, such as multipolar ordering including magnetic ones, heavy fermion behavior, intermediate valence state, and so on despite their simple NaCl crystal structure. Among them Ho monopnictide, HoX_p has not been studies intensively using a single crystalline sample because of the difficulty of its crystal growth. Among them, HoSb exhibits an antiferromagnetic transition of $T_N = 5.2$ K and is expected to be a well-localized 4*f* electron system. [2] To gain further knowledge on the ground state property and the nature of its bulk and surface states we performed ultrasound measurements on HoSb. In this study, we give results and possible interpretation of the elastic properties of HoSb as a function of temperature (T) and magnetic field (H), c_i (T, H).

Figure 1 shows an overall view of the temperature dependence of the longitudinal elastic constant c_{11}. A strong elastic softening was observed clearly toward the magnetic transition temperature T_N. The elastic constant behavior in this temperature region can be explained well by magnetoelastic effects due to the crystalline electric field effect of Ho^{3+} ions. From the results of various temperature and magnetic field scans, we summarized them in the $H - T$ phase diagram. In this talk, we discuss the elastic property, and also the nature of the order parameter in connection with the non-trivial topological property derived from its Dirac-cone-shaped band structure.

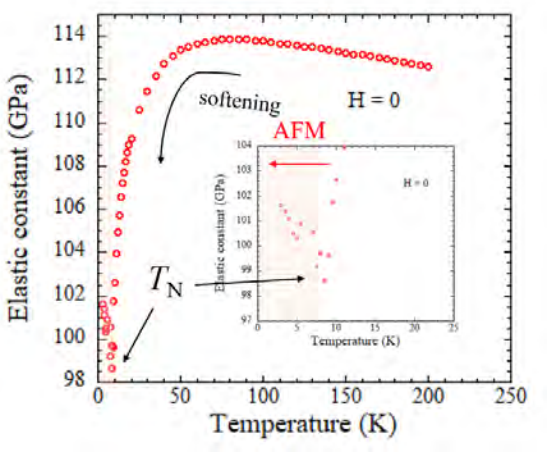

Fig.1. Temperature dependence of the elastic constant c_{11} in HoSb

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Ultrasound investigation of the Eu-based mixed valence system $EuRh_2Si_2$

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It is well-known that some Eu-based compounds exhibit valence instability and valence transition, depending on externally control parameters such as temperature, external magnetic filed, and pressure. Their systems are expected to be located on the border of a valence instability. In Eu-based compounds, valence fluctuation arises between divalent Eu (Eu^{2+}: $4f^7$, $J = 7/2$) and trivalent Eu (Eu^{3+}: $4f^6$, $J = 0$) ions. The Eu mean valence changes drastically in some cases, driven by the above external parameters. This situation provides a unique type of ground states, ranging from trivalent Eu showing Van Vleck susceptibility at low temperature to mixed valent state and finally divalent Eu, showing magnetic order at low temperature as in the homologous Gd compounds. In recent years there has been a growing interest in the physical properties of Eu-based compounds since their anomalous properties have been found to be associated with valence fluctuation, heavy fermion behaviour, and non-Fermi liquid (NFL) behaviour. Furthermore, the discovery of the topological properties including the novel surface state of some Eu-based systems stimulated the interest of researchers.[1] Motivated by these experiments, a great deal of effort has been devoted to understanding those exotic state observed in Eu-based compounds. Among Eu-based compounds, the $EuTr_2Si_2$ (Tr: transition element) series are in particular studied intensively so far. The observed ground state evolves systematically with the position of the Tr-element in the periodic table, from trivalent to divalent as one moves from left to right or top to bottom. Since unusually high magnetic ordering temperature of $T_N \sim 37$ K in $CeRh_2Si_2$ and NFL behaviour were discovered in $YbRh_2Si_2$, [2, 3] one can highly expect to find interesting magnetic behaviour also in $EuRh_2Si_2$.

$EuRh_2Si_2$ with the $ThCr_2Si_2$-type tetragonal structure is known as a pressure-induced valence transition compound.[4, 5] At ambient pressure, $EuRh_2Si_2$ exhibits antiferromagnetic ordering with a Néel temperature T_N of 25 K, and the Eu ion is in the divalent state.[6] The application of pressure first increases the Néel temperature T_N slightly and then causes the sudden collapse of antiferromagnetic state simultaneously with the occurrence of first-order valence transition at $P \sim 1$ GPa.[4, 5] To gain further knowledge on the ground state property we performed ultrasound measurements on the Eu-based mixed valence system $EuRh_2Si_2$. In this study, we give results and possible interpretation of the elastic properties of polycrystalline $EuRh_2Si_2$ as a function of temperature (T) and magnetic field (H), c_i (T, H). A polycrystalline sample of $EuRh_2Si_2$ was prepared by arc-melting constituent elements under an Ar atmosphere. Since no single crystal is available for this compound so far, we could measure the only experimentally accessible modes, i.e., the longitudinal and shear elastic constants (c_L and c_T). A tiny but clear anomaly of dip was observed in the both elastic constants at a T_N of 25 K. Besides, a faint anomaly was also recognized at $T^* \sim 10$ K in the both elastic constants. Interestingly, the both anomalies are strongly dependent on the external magnetic field strength. They both are suppressed rapidly with increasing a magnetic field and become invisible above a weak field of ~1 T. From the results of various temperature and magnetic field scans, we summarized them in the $H - T$ phase diagram. In this talk, we discuss the elastic property, and also the nature of the order parameter and some types of possible phases in $EuRh_2Si_2$ at low temperatures, in connection with the non-trivial topological property derived from its Dirac-cone-shaped band structure.

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Low-temperature x-ray crystal structure analysis of MBe$_{13}$ system

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The beryllides MBe$_{13}$ (M = rare earths and actinides) crystallize in a NaZn$_{13}$-type cubic structure with $Fm\bar{3}c$ (No. 226, O_h^6), which can be categorized as a cage-structured compound [1,2]. The M atoms in the 8a site are surrounded by 24 Be^{II} atoms in the 96i site, nearly forming an ideal snub cube, whereas the Be^{I} atoms in the 8b site are surrounded by 12 Be^{II} atoms, forming an icosahedron cage. In the present study, powder x-ray diffraction (XRD) measurements have been performed on LaBe$_{13}$, SmBe$_{13}$, and UBe$_{13}$ in the temperature range between 7 and 300 K in order to investigate their structure parameters at low temperatures and characteristics of a low-energy phonon which may be attributed to their unique caged structures [3,4].

For all three compounds investigated here, we estimated their Debye temperature to be 600 - 800 K from analyses of the temperature dependence of a lattice parameter, being in good agreement with the values reported previously [4,5]. In addition, Rietveld analyses of the obtained XRD patterns revealed that the M atom is located in the almost ideal snub cube formed by 24 Be^{II} atoms, whose caged structure is unchanged even at the low temperatures. Furthermore, it is argued from the temperature variation of an isotropic mean-square displacement parameter U_{eq} that the low-energy phonon for the present systems can be described well by a model assuming a conventional harmonic Einstein oscillation of the M atom with a characteristic temperature θ_E of ~ 160 K. Thus, the present study provides crystallographic collateral evidence for the presence of the low-energy phonon modes common to the MBe$_{13}$ systems [6]. Interestingly, the obtained θ_E values in the present systems, including the values reported thus far, appear to be independent of either mass of the guest atom or guest free distance r_{gfd} in the snub cube, as shown in Fig. 1, which is a characteristic feature not found in other cage-structured compounds.

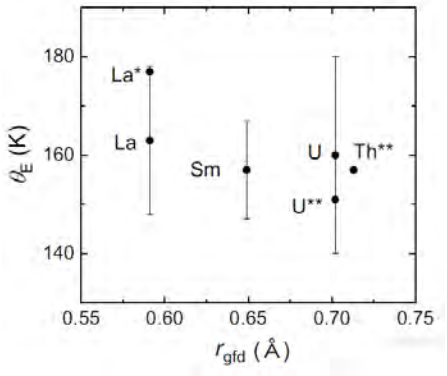

Fig. 1. Einstein temperature θ_E vs. guest free distance r_{gfd} (= $r_{M\text{-}BeII}$ - r_M - r_{BeII}) in several MBe$_{13}$ compounds, where M = La, Sm, Th, and U. Some data of θ_E, represented as La*, U** and Th**, are taken from literatures [3, 4].

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Split Fermi-Surfaces in Noncentrosymmetric Yb_4Sb_3

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We report the de Haas-van Alphen (dHvA) effect of noncentrosymmetric Yb_4Sb_3. Theoretically expected electronic structure consists of pairs of split Fermi surfaces (Fig.1) due to the antisymmetric spin-orbit interaction (ASOI) [1,2]. We found multiple, more than two, dHvA signals from some of the pairs. We attribute them to the result of orbital crossing at degenerate points of the split Fermi surfaces. There are two paths of carrier: one is intersecting and the other is passing-through the crossing (degenerate) point. In the latter path, the spin flip will take place at the crossing points. Strikingly, the probability of the intersecting is different in each Fermi-surface pair and field-direction. This result suggests that a novel transport property related to the spin structure characterized by the ASOI is realized in Yb_4Sb_3.

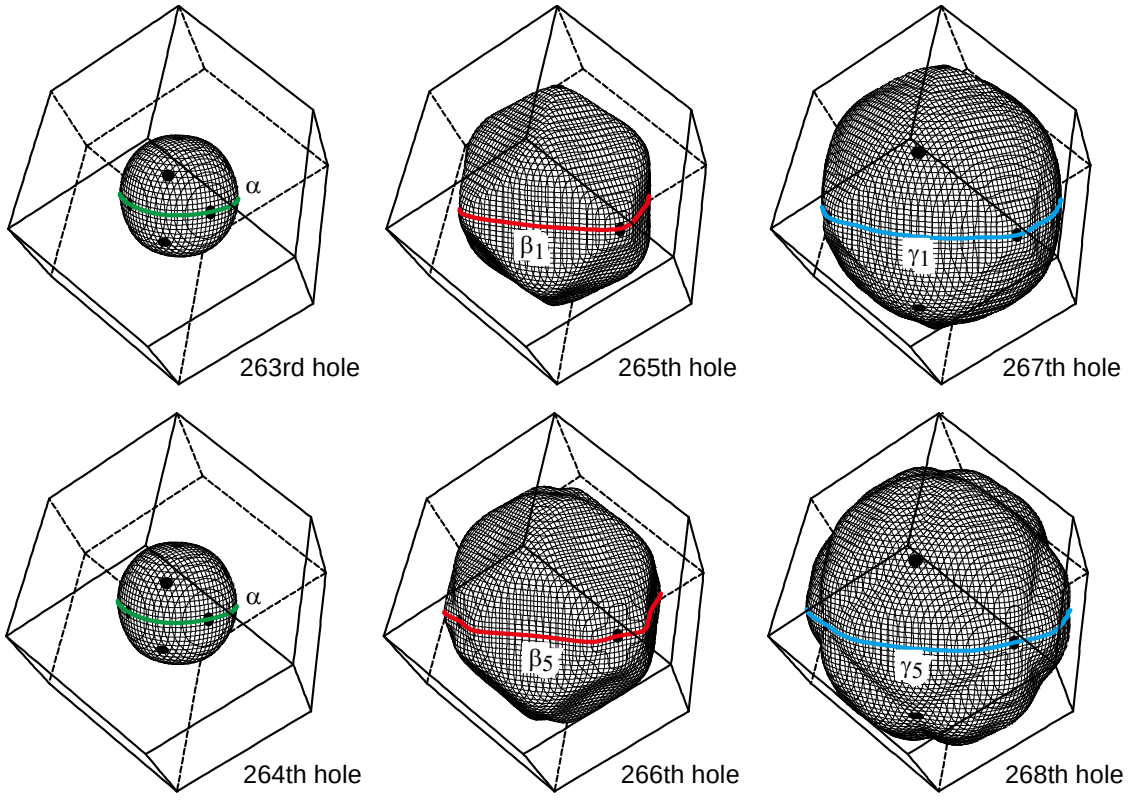

Fig. 1. Fermi surfaces of Yb_4Sb_3 obtained from the band structure calculation. Degenerate points are indicated by the black dot. The colored orbits correspond to the dHvA branches for the field along the <100> direction.

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Nonmagnetic doublet ground state of a cubic system $PrMgNi_4$

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Recently there has been considerable interest in cubic praseodymium-based compounds with non-Kramers doublet ground states of $4f^2$ configuration, because they show a variety of phenomena originating from quadrupolar degrees of freedom. For example, $PrPb_3$ shows an antiferroquadrupole (AFQ) order at $T_Q = 0.4$ K [1], below which the electric quadrupoles are aligned with a sinusoidally modulated structure [2]. In PrT_2Zn_{20} (T = Rh and Ir) and PrT_2Al_{20} (T = Ti and V), coexistence of quadrupole order and superconducting state was observed, suggesting that the quadrupole fluctuations may play a role in formation of the superconducting pair [3]. Moreover, PrT_2Zn_{20} (T = Rh and Ir) show non-Fermi liquid behaviors of the specific heat and the electrical resistivity at moderately wide temperature range above T_Q, where the anomalous temperature variations can be explained by a theoretical calculation with a two-channel Anderson lattice model [4].

In the present work, we have measured the electrical resistivity ρ, magnetic susceptibility χ, and specific heat of a Pr-based intermetallic compound $PrMgNi_4$ crystallizing in the cubic $MgSnCu_4$-type structure. Since the Pr-ion sits at a cubic T_d site, it is expected that the crystalline electric field (CEF) ground state could be the non-Kramers doublet with the active quadrupoles. The data of ρ measured for a polycrystalline sample decreases on cooling and shows a broad shoulder at around 12 K. χ follows the Curie-Weiss law, where the effective magnetic moment μ_{eff} and the paramagnetic Curie temperature θ_p was estimated to be $\mu_{eff} = 3.78\ \mu_B$/Pr and $\theta_p = -19$ K, respectively. On cooling for $T < 5$ K, χ approaches a constant value, indicating a Van-Vleck paramagnetic state. The magnetic specific heat C_m shows a broad maximum at around 4 K, which can be well reproduced by a two-level model with the ground state doublet and an excited triplet with an energy gap of 12 K. Thereby, it could be concluded that the CEF ground state of $PrMgNi_4$ is the non-Kramers doublet.

For the non-Kramers doublet ground state, it was expected that the active quadrupoles could play an important role for lifting the entropy of the ground state doublet. However, no phase transition was observed down to the lowest temperature of 0.08 K. Instead, on cooling for $T < 0.4$ K, the data of C_m approach a constant value. This behavior can be reproduced by a random two-level model on the assumption that the splitting energy is uniformly distributed by 5 K. Taking the random two-level state with no phase transition into consideration, the degeneracy of the doublet ground state must be split by symmetry lowering of the Pr site due to possible atomic disorder. Since the Pr and Mg atoms sit at the sites with the same point group, they may be randomly exchanged, leading to a non-magnetic singlet ground state with no active quadrupoles.

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Peculiar Magnetization Reversal of $TbNiC_2$

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$TbNiC_2$ has attracted much attention because of its rich and interesting properties of spin and charge ordering. It crystallizes in a noncentrosymmetric *A*-centered orthorhombic $CeNiC_2$-type structure with a space group *Amm*2 (C_{2v}^{14}, No. 38) [1]. The system exhibits a charge density wave (CDW) order with an incommensurate propagation vector $\boldsymbol{q}_1$ of (0.5, η, 0) at 243 K and two successive commensurate ones with $\boldsymbol{q}_{1C}$ of (0.5, 0.5, 0) and $\boldsymbol{q}_2$ of (0.5, 0.5, 0.5) at 160 K and 128 K, respectively. The commensurate CDW ordering state with $\boldsymbol{q}_{1C}$ persists even when the system undergoes an antiferromagnetic (AFM) transition at $T_N = 25$ K [2]. The reported magnetic structure is a noncollinear type described by the same propagation vector as $\boldsymbol{q}_{1C}$ with the Tb moments of 6.8 μ_B, where Tb moments are canted by about 13° from the *c* axis and by about 7° from the *b* axis [3,4]. The above-mentioned multiple phase transitions in $TbNiC_2$ imply an intriguing interplay between CDW and AFM [2]. Moreover, the system exhibits a weak spontaneous magnetization *M* of about 0.22 μ_B in the AFM state [5]. Although the above-mentioned magnetic structure cannot explain this weak ferromagnetic component, there are few studies in low-magnetic fields thus far. We thus focus on the magnetic response to low-magnetic fields in order to reveal the origin of the weak ferromagnetism of this system.

In the present study, the magnetization for the single-crystalline samples of $TbNiC_2$ along different field directions were measured in the temperature range from 2 to 300 K with applied magnetic field up to 15 kOe. Figure 1 shows *M* as a function of temperature upon field cooling (FC) in various magnetic fields along the *c* axis. We found that *M* in the FC process decreases below T_N across zero with decreasing temperature, and becomes negative with fields lower than 500 Oe. It is revealed that this unusual "magnetization reversal" occurs only below T_N and only in the FC process. As can be seen in Fig. 2, it is clear that the observed magnetization reversal is not due to a conventional diamagnetism such as the core diamagnetism or Landau diamagnetism since the differential susceptibility is always positive. We will discuss the origin of this peculiar magnetization reversal of $TbNiC_2$.

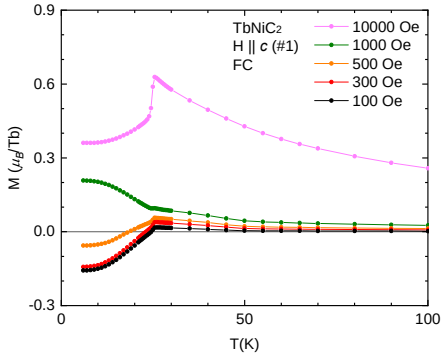

Fig. 1. Temperature dependences of the magnetization upon FC in various magnetic fields along the *c* axis.

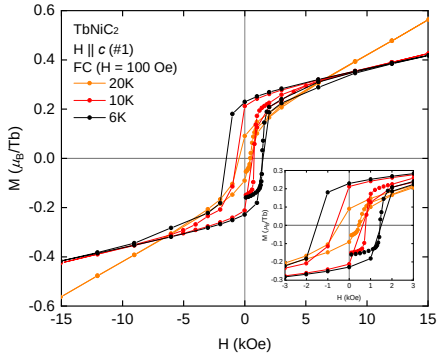

Fig. 2. Isothermal magnetization processes measured at several temperatures for magnetic field along the *c* axis after FC at 100 Oe.

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Ground-state 4f orbital symmetry probed by linear dichroism in core-level photoemission spectra of strongly correlated Sm compounds

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Rare earth-based strongly correlated electron systems show various interesting behavior, for example, formation of heavy fermion, superconductivity, and magnetic/multipolar ordering. Since such phenomena are seen at low temperatures, the information of rare-earth 4f ground-state symmetry is important to clarify mechanisms for these interesting phenomena.

So far we have revealed that anisotropic 4f charge distributions due to the crystalline electric field are responsible for linear dichroism (LD) in 3d core-level photoemission spectra of rare earth compounds. Indeed, the crystal-field ground-state 4f symmetry has been clarified by successfully observed LDs in some of the rare-earth compounds [1-4]. We have also observed LDs in Sm^{3+} $3d_{5/2}$ photoemission spectra of tetragonal $SmCu_2Si_2$ [5]. However, the perfect determination of its crystal-field ground-state symmetry was difficult because of the characteristic Sm^{3+} 4f charge distribution (see Fig. 1).

Therefore, we have observed LDs in the Sm^{3+} $3d_{5/2}$ photoemission spectra of tetragonal $SmCu_2Si_2$ at two significantly different photoelectron directions far from the c axis. The obtained polarization-dependent Sm^{3+} $3d_{5/2}$ core-level photoemission spectra and LDs with the simulated LDs for the Γ_7^1 and Γ_7^2 ground state are shown in Fig. 1. The LDs of $SmCu_2Si_2$ are well reproduced by the simulations for the Γ_7^1 states rather than those for the Γ_7^2 states, from which the Sm^{3+} 4f ground state of $SmCu_2Si_2$ in the $\Gamma_7^1 >= \sqrt{0.6}\,|\pm 5/2> -\sqrt{0.4}|\mp 3/2>$ symmetry is established.

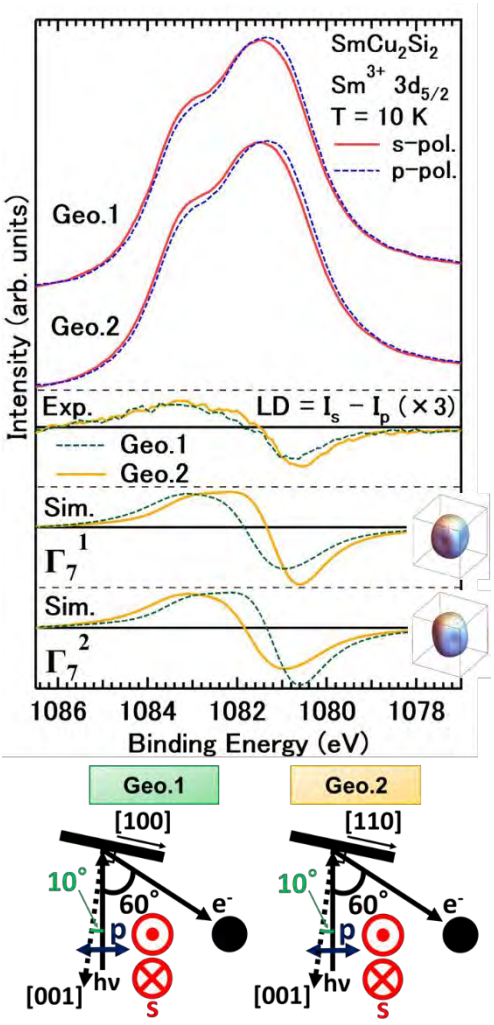

Fig. 1. Polarization-dependent Sm^{3+} $3d_{5/2}$ core-level photoemission spectra and LDs of tetragonal $SmCu_2Si_2$ with the simulated ones for the Γ_7^1 and Γ_7^2 ground state with the experimental geometry. The likely 4f charge distributions are also shown.

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^{151}Eu Mössbauer Spectroscopy of Chiral Antifferomagnet EuPtSi

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Trillium with three white petals arranged symmetrically (fig. 1) is well known as the provincial flower of Ontario, Canada. The trillium lattice, a tree-dimensional network corner-sharing triangles resembling a trillium flower appears in some cubic compounds crystalizing with space group $P2_13$, where atoms locates at 4*a* sites of the .3. site symmetry. A new type of topological magnetic texture so called the magnetic skyrmion was discovered in in the A-phase under the magnetic fields just below the Néel temperature T_N of the B20-type helimagnets such as MnSi and FeGe having the trillium lattice. The trillium lattice is also realized in EuPtSi intermetallic compounds of LaIrSi type structure as shown in fig. 2. Recently, Kakihana *et al.*[1] and D.G. Franco *et al.*[2] observed the first-order like antiferromagnetic ordering of EuPtSi at T_N=4.0 K, which are small in magnitude compared with ordering temperatures of 10–100 K in the usual divalent Eu compounds, reflecting the frustration of spins in the chiral structure. A magnetic Phase diagram of EuPtSi including the A-Phase was determined by the Hall resistivity and the magnetization.[3] However, microscopic study of EuPtSi has been performed for only above 4.2 K by Mössbauer spectroscopy[4]. We measured the ^{151}Eu Mössbauer spectra of EuPtSi between 3.06 and 300 K. A symmetrical Lorentzian absorption of the paramagnetic states turns to the magnetic splitting profile below 4.0 K as shown in fig. 3. Spectrum at 3.9 K consists of sum of the paramagnetic and the magnetic states indicating the first-order like ordering at T_N=4.0 K. But the half width of symmetrical Lorentzian absorption is previously broadened below 8 K. These results correspond the reported magnetic entropy reaching *R*log8 at around 10-15.

Fig. 1. Illustration of Trillium Flower.

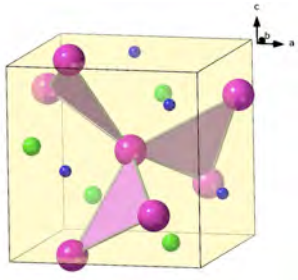

Fig. 2. Crystal Structure of EuPtSi.

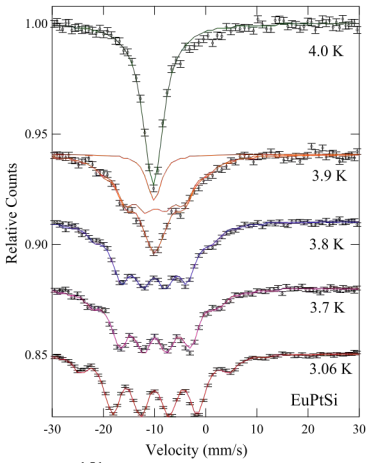

Fig. 3. ^{151}Eu Mössbauer Spectra of EuPtSi below 4 K.

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Heavy fermion state of $YbNi_{1.8}Si_{3.2}$ without local inversion symmetry

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Recently, globally or locally non-centro-symmetric crystals have been attracted, because novel physical phenomena, such as chiral magnetism [1-3], magnetoelectric effects [4-6], and anisotropic superconductivity [7, 8], appear. In the crystals without local inversion symmetry, antisymmetric spin-orbit couplings occur, but it is heterogeneous in the unit cell because of macroscopic preservation of space inversion symmetry. A paramagnetic cooper-pair breaking effect often becomes small owing to the antisymmetric spin-orbit couplings in this system, indicating that a superconducting state can be realized in higher temperature (magnetic field) [9]. There are not many examples showing superconductivity with such feature. On the other hand, the local inversion symmetry is broken in high temperature superconductors such as Iron-based and copper oxide superconductors. The local inversion symmetry breaking may cause high superconducting critical temperature. In order to clarify physical phenomena owing to local inversion symmetry breaking, it is important to study antisymmetric spin-orbit couplings, which becomes easier to observe in lower temperature range. Therefore, it is one of meaningful subject of study to investigate crystals whose local inversion symmetry is broken, which may cause unconventional superconductivity with heavy fermion at very low temperature.

We have succeeded to grow a single crystalline heavy fermion compound $YbNi_2Si_3$ by means of Sn-flux method with the size of 0.5~3 mm. We have decided the crystal structure of $YbNi_2Si_3$ as $ScNi_2Si_3$ type crystal structure (space group: *I4/mmm,* No. 139) by using X-ray structural diffraction. The crystal structure of $YbNi_2Si_3$ is interesting, because there is no local inversion symmetry at Yb site, which plays a role of magnetism, whereas the unit cell has inversion symmetry. We have also conducted composition analysis by EPMA. As a result, there are some variations in the composition, and it turned out that the average value is Yb:Ni:Si=1:1.8:3.2, suggesting that there are some defect of Ni and excessive of Si in this compound. The composition variation has little influence on the magnetization, so we have measured the magnetization and specific heat with the average composition $YbNi_{1.8}Si_{3.2}$. At zero field, specific heat of this sample shows a peak at $T_N \sim 0.3$ K (see Fig.1). Surprisingly, a large value of $(C\text{-}C_{nuc})/T \sim 5$ J/mol K^2 remains even at very low temperature ~ 0.08 K. This result suggests that heavy fermion state is realized at very low temperature, and an additional phase such as unconventional superconductivity is expected in ultra-low temperature region below 0.08 K.

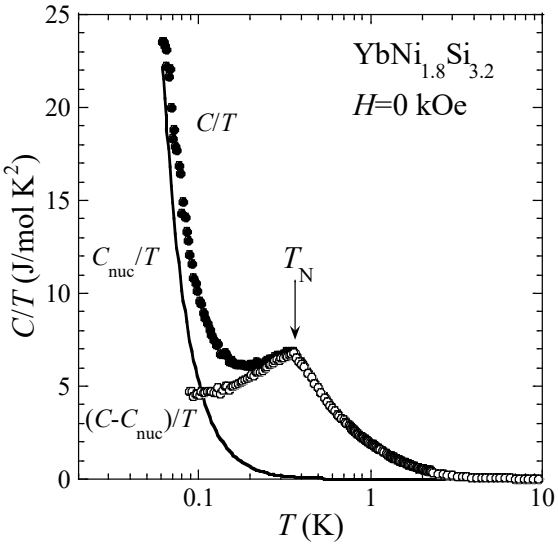

Fig. 1. Specific heat of $YbNi_{1.8}Si_{3.2}$ at zero field. C/T is the raw specific heat, C_{nuc}/T is a fitting result of C/T with a function of A/T^3, $(C\text{-}C_{nuc})/T$ is a difference between C/T and C_{nuc}/T, and T_N is Néel temperature.

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Synchrotron-radiation-based ^{174}Yb Mössbauer spectroscopic studies on $YbAlB_4$

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Valence fluctuating compounds α- and β-$YbAlB_4$ with valences of $Yb^{+2.7}$ [1] have orthorhombic structures at ambient conditions. These structures are layered ones consisting of alternate stacking of the Yb and Al layers with the B layers along the *c*-axis with one Yb crystallographic site, in which the local structures at the Yb ions are similar in α- and β-$YbAlB_4$. α-$YbAlB_4$ forms a heavy-Fermion state below T^*~8 K [2] in spite of a mixed valence state. We have studied the effects of external magnetic field for α-$YbAlB_4$ with the heavy-Fermion state by ^{174}Yb Mössbauer spectroscopy and x-ray diffraction using synchrotron radiation.

We have carried out ^{174}Yb synchrotron-radiation-based Mössbauer and x-ray diffraction measurements for α-$YbAlB_4$ at low temperature on the BL09XU and BL19XU at SPring-8, respectively. In the Mössbauer spectroscopy, the spectra were accumulated at 2 K with external magnetic fields range from 0 to 60 kOe, where the directions of incident x-ray with the σ-polarization and external magnetic fields were along the *c*-axis of the single-crystalline sample. In the x-ray diffraction using the single-crystalline sample, several (*h k* 0) diffraction lines were measured at 2 K up to 60 kOe, where the external magnetic field was also applied long the *c*-axis.

The observed ^{174}Yb Mössbauer spectra at 2 K exhibit drastically change in its characteristic feature at ~ 20 kOe and 2 K with increasing external magnetic field, revealed change of the hyperfine interactions at ^{174}Yb nuclei in α-$YbAlB_4$. We have analyzed these observed spectra, assuming that one of the principle axes of the hyperfine interactions is along the *c*-axis form the local symmetry, ..*m*, at the Yb ions in α-$YbAlB_4$. The analytical spectra well reproduce these observed one except for the spectrum at 20 kOe and 2 K. The extracted magnetic hyperfine field is the same as the external magnetic field with our experimental accuracy, indicted that there is negligible small contribution in the magnetic hyperfine field from the 4*f* electron of Yb ions. Our analyses reveal that the principle *z* axis of the electrical quadrupole interaction changes in the *c* plane. Furthermore, the external magnetic field dependence of the refined isomer shift changes around ~20 kOe.

The refined *d*-values of the (0 6 0), (0 10 0), (1 11 0), and (2 15 0) diffractions lines maintain up to 60 kOe at 2 K, indicated that the orthorhombic symmetry and the *a* and *b* lattice parameters of α-$YbAlB_4$ do not change by the external magnetic field. Meanwhile, these integrated intensities exhibit anomaly at ~ 20 kOe and 2 K. Although the intensity of the (1 11 0) diffractions line is small within the kinematic conditions, the intensity maintains up to 20 kOe and then decrease with increasing external magnetic field. These results reveal that the local structure at the Yb site is changed by the external magnetic field without the structural transition.

This magnetic field, 20 kOe at 2 K, corresponds to the anomaly in external magnetic field dependence of the electrical resistivity [3]. In a rear-earth ion where the total angular momentum is a good quantum number, the electrical quadrupole interaction is mainly due to contributions from the nonspherical 4*f* electron distribution. The change of the principle axes of the electrical quadrupole interaction is related to that of the nonspherical 4*f* electron distribution due to the local structure at the Yb site in α-$YbAlB_4$.

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Theory for anomalous temperature dependence of relaxation rate measured by μSR in α-$YbAl_{0.986}Fe_{0.014}B_4$

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It was reported by MacLaughlin *et al*. [1] that α-$YbAl_{0.986}Fe_{0.014}B_4$ exhibits an anomalous temperature dependence in the μSR elaxation rate $1/T_1$, as shown in Fig. 1, and stressed that the temperature dependence $1/T_1 \propto T^{-0.4}$cannot be understood by the scenario based on the quantum critical valence transition (QCVT) while this compound exhibits a series of the non-Fermi liquid behaviors [2] explained quite well by the theory of the QCVT [3,4].

In this presentation, we show the anomalous temperature dependence in $1/T_1$ can be understood semi-quantitatively by taking account of the effect of the μ^+ that extracts conduction electrons around it, and in turn induces the local magnetic moment arising from 4f- hole on Yb ion, giving rise to the Kondo effect between heavy quasi-particles.

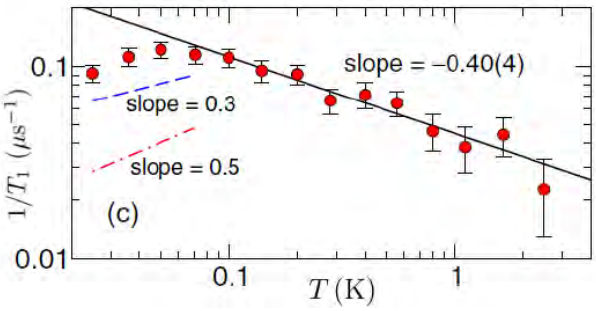

Fig. 1 Temperature dependence of μSR relaxation rate $1/T_1$ [1].

The anomalous exponent α (defined as $1/T_1 \propto T^{-\alpha}$) arises from that of the renormalized exchange coupling $J_{qf}(T)$ between 4f-hole on Yb and renormalized quasiparicles of mother compound α-$YbAl_{0.986}Fe_{0.014}B_4$ in the region $T > T_K$ (with T_K being the Kondo temperature of the Kondo effect between local moment induced on Yb site and quasiparticles of mother compound). The temperature dependence of $\alpha(T)$ can be determined by the two-loop order renormalization group calculation (valid at $T > T_K$) as shown in Fig. 2, reproducing T dependence in $1/T_1$ (at $T > 0.1$ K) shown in Fig. 1. Vertical dashed line shows the Kondo temperature T_K (in the unit of effective band width of quasiparticles D^*) which gives $\alpha(T) = 0.4$ (observed value in the region $T >> T_K$). D^* is estimated as $D^* = 30$K form the T dependence of the specific heat of mother compound [5]. Then, in turn, the Kondo temperature of T_K of the present problem is estimated as $T_K = 0.2$ K below which the effect of Kondo-Yosida screening starts to work recovering the exponent of the relaxation rate $1/T_1 \propto T^{0.5}$ ($>> T$) predicted by the theory of QCVT [3].

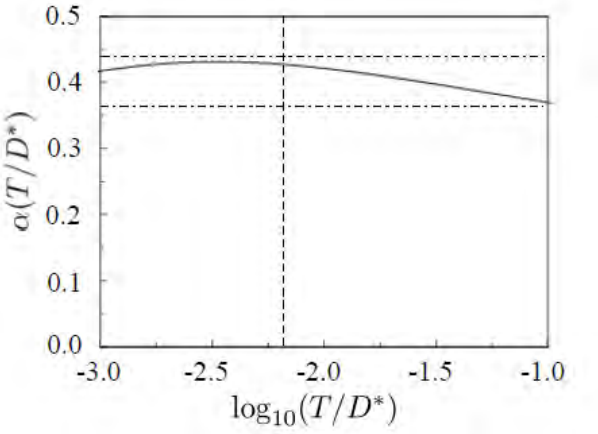

Fig. 2 T dependence of anomalous exponent $\alpha(T)$.

Thus, the anomalous T dependence in $1/T_1$ shown in Fig. 1 is explained semi-quantitatively.

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Quantum criticality induced by magnetic field in the cage compound PrV_2Al_{20}

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The group of isostructural intermetallic ternaries with the general formula RTr_2X_{20} (R = rare earths and uranium, Tr = transition metals, X= Al, Zn, and Cd), so-called 1-2-20 systems has attracted considerable attention and been extensively studied in the past decade since they manifest a diverse range of novel quantum phenomena at low temperatures, such as heavy fermion (HF) behavior with a gigantic value of its Sommerfeld coefficient γ (effective mass), non-Fermi liquid behavior, multipole ordering and unconventional superconductivity. It is believed that they are mainly driven by the relatively large hybridization between conduction and 4f electrons including quadrupole (orbital) moments or/and multipole ones. In particular, the Pr-based 1-2-20 systems with the non-Kramers Γ_3 ground state doublet, would be an interesting playground in which to address quantum criticality associated purely with quadrupolar/orbital degrees of freedom.

PrV_2Al_{20} crystallizes in the cubic $CeCr_2Al_{20}$-type structure (space group: $Fd\bar{3}m$, No. 227) in which Pr ions are encapsulated in the Frank-Kasper cages formed by sixteen neighboring Al ions. Pr and V atoms form a diamond structure and a β- pyrochlore type partial sub-lattices, respectively. PrV_2Al_{20} exhibits quadrupolar ordering at T_Q = 0.65 K and heavy fermion superconductor with T_c = 50 mK at ambient pressure.[1-2] Furthermore, additional ordering was recently discovered at 0.75 K. We have clearly observed elastic anomalies in the temperature dependence of principal elastic constants at the ordering temperatures of 0.65 K and 0.75 K.[3] Based on the experimental data, magnetic field vs temperature phase diagram was constructed for PrV_2Al_{20}. The obtained result provides an extended insight into the fundamentals of a quadrupolar ordering derived from the non-Kramers doublet Γ_3. Furthermore, a pronounced elastic softening toward low temperature is revived by applying a magnetic field in the temperature dependence of the elastic constant $(C_{11}\text{-}C_{12})/2$, due to the non-Kramers doublet Γ_3, being degenerate in the order parameter space (O_{20}, O_{22}) .[4] we conducted further the ultrasound measurement on PrV_2Al_{20} under the external magnetic field applied along the <111> crystallographic axis.

In this talk, we discuss the field-tuned quantum criticality based solely on the quadrupolar degrees of freedom through the evolution with magnetic fields applied along the <111> crystallographic axis, combined with the previous data under the external magnetic field applied along the <100> and <110> crystallographic axes.

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Quadrupole order in 1-2-20 system based on first-principles calculations

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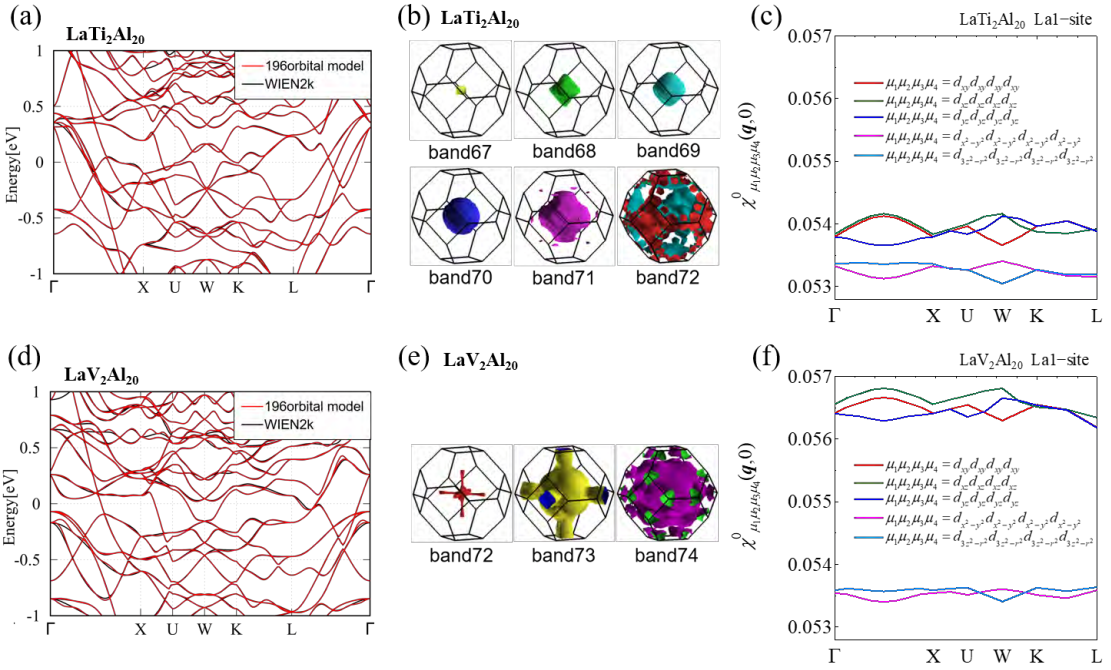
Recently, Pr 1-2-20 systems (PrT_2X_{20}) have attracted much attention as they exhibit various quadrupole orders, e. g. the ferro-quadrupole order (FQ) in $PrTi_2Al_{20}$ and the antiferro-quadrupole order (AFQ) in PrV_2Al_{20}, $PrIr_2Zn_{20}$ and $PrRh_2Zn_{20}$, and also exhibit the superconductivity which is found to show a close relationship with the quadrupole order [1]. The CEF ground state of Pr^{3+} ion in Pr 1-2-20 is considered to be the non-Kramers doublet Γ_3 state with the quadrupole moment. According to the experiment of de-Haas van Alphen (dHvA) effect, the Fermi surfaces of the Pr 1-2-20 are similar to those of the corresponding La 1-2-20 [2,3]. Therefore, the $4f^2$ electrons of Pr^{3+} ion do not participate in the Fermi surfaces and then are considered to be localized yielding the localized quadrupole moments. In this case, the Ruderman-Kittel-Kasuya-Yoshida (RKKY) interaction between the quadrupole moments between the neighbouring Pr ions is crucial to determine which types of quadrupole orders (FQ or AFQ) are realized in each compounds [4]. However, the explicit calculation of the RKKY interaction in the Pr 1-2-20 has not been performed so far. The purpose of this study is to obtain the RKKY interaction on the basis of the first-principles band calculations for various 1-2-20 systems and to discuss the quadrupole orders. We show some obtained results in Fig. 1: the energy bands from the first-principles calculations (WIEN2k) together with those from the effective 196 orbital model derived by the maximally localized wannier functions (Wannier90) for $PrTi_2Al_{20}$ and PrV_2Al_{20} in Figs. 1 (a) and (d), respectively, the corresponding Fermi surfaces in Figs. 1 (b) and (e), and the several components of the orbital susceptibilities from the 196 orbital model in Figs. 1 (c) and (f), where we see distinct differences between the two compounds.



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Ultrasonic measurements on the cage compound $SmPt_2Cd_{20}$

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The class of compounds known as so-called 1-2-20 systems, crystallizing in a cubic $CeCr_2Al_{20}$ – type crystal structure exhibits a wide variety of strongly correlated electron phenomena including multipolar ordering, the related Kondo effect and super heavy fermion behavior. In particular, magnetically robust heavy fermion state formed in some Sm-based 1-2-20 systems is one of the interesting and central issues to be studied in the strongly correlated electron systems. $SmPt_2Cd_{20}$ is known to undergo phase transition below 0.64 K without the presence of a magnetic anomaly in its magnetic susceptibility. The temperature dependence of the electrical resistivity shows a shoulder-like structure around 10 K, possibly due to the reduction of crystalline electric field (CEF) excitation of 4*f* electrons. It might be inferred that the CEF splitting would be small. The temperature dependence of the magnetic resistivity, estimated by subtracting the resistivity of a proper isostructural reference $LaPt_2Cd_{20}$ from that of $SmPt_2Cd_{20}$ slightly increases with decreasing temperature. This is likely to be due to the logarithmic temperature dependence, implying Kondo-like behavior. The low temperature Sommerfeld specific heat coefficient C_{4f}/T is estimated to be 4.5 J/(mol K^2), strongly indicating the development formation of heavy fermion particles. [1, 2] However, the mechanism responsible for the enhancement of effective mass is still a puzzle. On the other hand, hyperfine coupling between an electronic and a nuclear spin would be rather enhanced, with the consequence the heavy fermion state contains a large contribution from the nuclear state of Sm. We performed ultrasound measurements on $SmPt_2Cd_{20}$ in the extremely low temperature ranges covering the area mentioned above, using a ^{4}He refrigerator down to 1.4 K and a ^{3}He-^{4}He dilution refrigerator down to 80 mK. Superconducting magnets equipped with the refrigerators were employed for the ultrasonic measurements in applied magnetic fields.

Figure1 shows the low-temperature dependence of the relative change of the elastic constant c_{11} under the selected fields. The clear elastic softening behavior is suppressed gradually with increasing magnetic field. It should be noted here that an elastic anomaly due to the magnetic transition is recognized well. From the results of various temperature and magnetic field scans, we summarized them in the $H - T$ phase diagram as shown in Fig. 2. In this talk, the nature of the low temperature elastic properties and electronic states involving the ground state multiplets of Sm ions will be discussed.

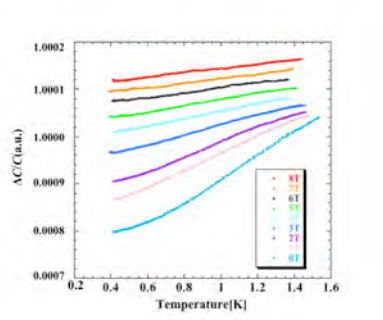

Fig.1 : Temperature dependence of elastic constant C_{11}

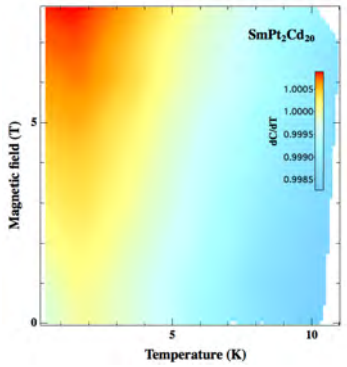

Fig.2 : magnetic phase diagram

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Neutron scattering and synchrotron x-ray diffraction study on PrTr_2Al_{20} (Tr = Ti, V)

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Non-magnetic PrTr_2Al_{20} (Tr = transition metals) has been attracting extensive interests recently, because of their intriguing low temperature anomalies [1]. For instance, $PrTi_2Al_{20}$ and PrV_2Al_{20} show clear anomalies at 2 K and 0.6 K in the specific heat measurements, nonetheless the magnetic susceptibility hardly detect such anomalies near zero field. As the crystal electric field ground state of Pr^{3+} in the PrTr_2Al_{20} compounds are suggested as the non-magnetic but quadrupolar- (and octapolar-) active Γ_3 state, these anomaly may be due to the ordering of quadrupolar degree of freedom. Magnetic susceptibility and electric resistivity in PrV_2Al_{20} show anomalous metallic behavior at low temperatures explained as $\chi \sim - T^{1/2}$ and $\rho \sim \ln T$, which are different from those of $PrTi_2Al_{20}$. In $PrTi_2Al_{20}$ and PrV_2Al_{20}, superconducting transitions are observed. Especially, in PrV_2Al_{20}, it is also found that the superconducting transition temperature strongly depends on the residual resistivity ratio of the sample [3].

To determine the ground state of the quadurpolar Kondo materials PrTr_2Al_{20}, the neutron scattering experiments were carried out [2]. The observed inelastic neutron scattering for PrV_2Al_{20} is obviously broader than that for $PrTi_2Al_{20}$. Thus, the strong *c-f* hybridization effect is expected in PrV_2Al_{20}. Next, the quadrupolar orderings have been concluded for $PrTi_2Al_{20}$ and PrV_2Al_{20} by observing the reduction of the intensity of the induced magnetic (2 2 0) reflection under the magnetic field. We also found the peculiar magnetic field dependence of (2 2 0) reflection in PrV_2Al_{20}. The observed intensity for PrV_2Al_{20} shows linear magnetic field dependence in the low magnetic field ($B < 2$ T) and low temperature ($T < 4$ K), while the magnetic field dependence of the induced magnetic reflection for $PrTi_2Al_{20}$ obeys a quadratic function B^2. This magnetic field dependence for PrV_2Al_{20} can be explained by the assumption that the free energy depends on $F \propto (B)^{3/2}$.

Next, to obtain the crystal structure information for $PrTi_2Al_{20}$ and PrV_2Al_{20}, the synchrotron x-ray diffraction experiments and crystal structure analyses were performed. We observed 4 % deficiency of Pr-site for PrV_2Al_{20}, in contrast with less than 1 % deficiency for $PrTi_2Al_{20}$. This Pr-site deficiency is possibly related to the change of the quadurpolar ordering and superconducting transition temperatures.

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Multipole order and non-Fermi liquid in quadrupole Kondo lattice PrV_2Al_{20}

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The cubic $PrTr_2Al_{20}$ (*Tr* = Ti, V) is an unique *quadrupolar* Kondo lattice system, where both strong *c-f* hybridization and nonmagnetic cubic Γ_3 CEF ground state are realized [1]. For $PrTi_2Al_{20}$, ferroquadrupole ordering at $T_Q = 2.0$ K is well established by various measurements such as specific heat, ultrasound, nuetron scattering and NMR[1-4]. In the ferroquadrupole ordered state, superconductivity is observd at $T_c = 0.2$ K with moderately enhanced effective mass $m^* \sim 20m_0$ [5]. T_c and m^* are highly enhanced to ~1 K and ~100 m_0 by the application of pressure due to the quantum criticality of ferroquadrupole ordering [6].

By replacing Ti to V, *c-f* hybridization can be stronger due to the chemical pressure and an additional electron. Indead, non-Fermi liquid behavior such as $\rho \sim T^{0.5}$ is observed even at ambient pressure. Quadruple order is suppressed and becomess double transition at $T_Q = 0.75$ K and 0.65 K [7]. So far, the origin of this double transition is not yet well understood.

In this presentation, we will show our recent results of thermal expansion and magnetostriction measurements and discuss the possible origion of the double transition.

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NMR structural analysis of single crystal UNi_4B

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UNi_4B exhibits an antiferromagnetic (AFM) ordering at T_N = 20 K and shows highly anomalous magnetic behaviour in the AFM state[1,2], where the uranium magnetic moment forms a vortex-like structure with multiple propagation vector Q in the [0001]-plane, so called a ferro-toroidal ordering [3]. In the early stage, the crystal structure of this material was reported to be the hexagonal $CeCo_4B$-type crystal structure described by the space group P6/mmm[1]. The magnetic structure reported in Refs.[1-3] is based on the above hexagonal crystal structure. However, the neutron scattering experiment on single crystal UNi_4B, it was also reported that weak superstructure reflections corresponding to an existence of a larger unit cell [2]. Haga and co-workers carried out single crystal X-ray diffraction study for a high-quality single crystal sample. They reported that the crystal structure is the orthorhombic with Cmcm space group [4]. Recent synchrotron X-ray experiments on single crystal UNi_4B have suggested that the crystal structure is orthorhombic structure with either Cmcm [4,5] or $Cmc2_1$ [5] space group.

Here we report ^{11}B-NMR results on single crystal UNi_4B. Since the ^{11}B nucleus has the quadrupole moment of $^{11}Q=0.04\times10^{-24}$ cm^2, then, ^{11}B-NMR line profile is sensitive for local symmetry at B site. That is, ^{11}B-NMR line profile should be different for each space group, i.e, a single NMR line is expected for the hexagonal P6/mmm space group, four NMR lines for the orthorhombic Cmcm space group, and six lines for orthorhombic $Cmc2_1$. In the previous meeting [6], we reported the results of the frequency-swept ^{11}B-NMR measurements. The obtained ^{11}B-NMR line profile cannot be explained by the hexagonal structure, but rather it can be explained by an orthorhombic structure with either Cmcm or $Cmc2_1$. However, the obtained ^{11}B-NMR spectrum cannot be distinguishable between above two space groups because of the weak signal to noise ratio of the NMR signals. In order to improve experimental precision, we utilized a fast-Fourie-Transform (FFT) NMR technique with the short excitation pulse width of 1μs. In this poster, we will report details of NMR structural analysis of UNi_4B.

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X-ray Crystal Structure Analysis of Toroidally Ordered System UNi_4B

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The interplay between electric and magnetic properties of electrons in matter has attracted much interest in recent condensed matter physics. In particular, the phenomena that magnetism couples with ferroelctricity, which is called the magnetoelectric (ME) effect, has been studied intensively since the discovery of multiferroic materials. The ME effect had been considered as a property that only insulating materials can exhibit, because metallic materials have no electric polarization. However, a recent theoretical study proposes that the ME effect can arise also in metals in which the magnetic moments order in vortex-like arrangements, referred to as toroidal order [1]. UNi_4B is the first example of toroidal ordering metal that is confirmed experimentally to exhibit magnetization induced by electric current [2]. The experiment and theory are, however, not fully consistent with each other about the directions of applied electric current and induced magnetization. One of problems that hinder understanding of this phenomena is the crystal structure of this compound. There are two controversial reports of crystal structure of this compound: the hexagonal (*P*6/*mmm*) [3] and orthorhombic (*Cmcm*) [4] ones, both of which were investigated using laboratory X-ray sources. We performed crystal structure analysis using high-energy synchrotron X-ray, in order to determine the crystal structure of UNi_4B.

A small piece (about 20 micron in diameter) of single crystalline UNi_4B grown by Czochralski method was used as a specimen. The diffraction of synchrotron X-ray was measured by using a diffractometer with an imaging-plate type detector at a beamline PF-AR NE1A in Photon Factory. The high energy X-ray of 30 keV was utilized to reduce the large absorption effect of the heavy U atoms in the sample. The obtained diffraction patterns strongly suggest the orthorhombic unit cell, whose lattice constants are: a = 6.922(4) Å, b = 14.773 (2) Å, c = 17.04 (1) Å, which is the same as the one of the previously reported structure [4]. The observed reflection conditions indicate possible space groups as follows: *Cmcm* (D_{2h}^{17}, no. 63), *Cmc*2$_1$ (C_{2v}^{12}, no. 36), and *C*2*cm* (C_{2v}^{16}, no. 40). The direct method using SIR2011 and the least-squares refinement using SHELX give very similar structures for each of these space groups, which have distorted triangular lattices formed by U atoms, without local inversion symmetry at each U site (see Fig. 1). The differences of *R*-values of the refinements among these space groups are no more than 0.5 %. In order to choose the correct space group out of these three candidates, we need careful check from other experimental methods that are sensitive to symmetry of the system, such as NMR, and so on.

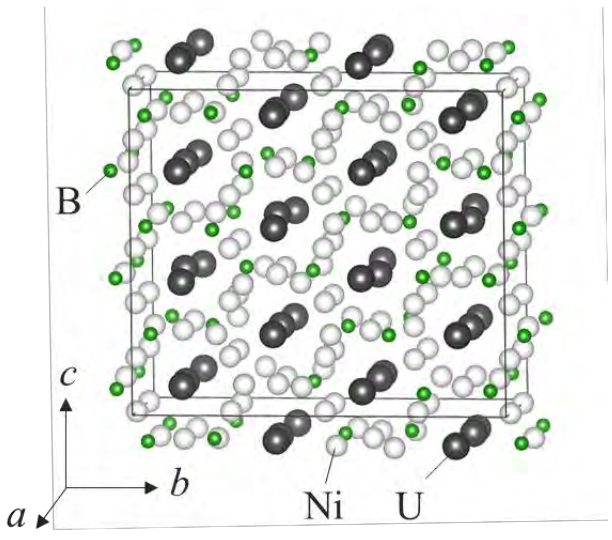

Fig. 1. Crystal structure of UNi_4B suggested by the least-squares refinement, assuming the space group of *Cmcm*.

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Paramagnetic electronic structure of UNi_4B

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Recently, current-induced magnetization in a metallic system lacking local-inversion symmetry has been observed in UNi_4B [1]. The crystal structure of UNi_4B was considered to be a hexagonal $CeCo_4B$-type crystal structure (#191, *P6/mmm*, D_{6h}^1), but has been discussed to be an orthorhombic, *Cmcm* (#63, D_{2h}^{17}) [2, 3] or $Cmc2_1$ (#36, C_{2v}^{12}) [3]. Therefore, the calculations are carried out for the reported crystal structure. Recent ^{11}B-NMR measurements strongly suggest that the crystal structure should be orthorhombic [4].

To investigate the electronic structure and EFG (Electronic Field Gradient) at B-site, electronic band structure calculations have been performed for UNi_4B and $ThNi_4B$ (U is just replaced by Th), by using an FLAPW method based on the LDA (Local Density Approximation). The calculations are done for paramagnetic cases. A primitive unit cell of the hexagonal UNi_4B contains 12 atoms, while the unit cell of the orthorhombic structures becomes 6 times larger, then contains 72 atoms. It means huge computer resources are necessary to get accurate results. Therefore, the results for UNi_4B and $ThNi_4B$ in the hexagonal structure, and the preliminary result for $ThNi_4B$ in *Cmcm* case have been obtained, so far. The calculated EFGs at B site are listed in Table. 1.

After comparing EFGs between UNi_4B and $ThNi_4B$ in a hexagonal case, the *5f* electrons on U do not affect so much the EFG at B site. In an orthorhombic *Cmcm* structure, B site splits to four crystallographically inequivalent sites. The calculated EFGs values are clearly scattered, then should be identified by experiments.

Table 1. Calculated EFG (converted to frequencies) and the anisotropic parameter η for the hexagonal UNi_4B and $ThNi_4B$ (#191, *P6/mmm*, D_{6h}^1) and the $ThNi_4B$ in *Cmcm* (#63, D_{2h}^{17}). There are four crystallographically inequivalent B sites in the *Cmcm* case.

	UNi_4B	$ThNi_4B$	$ThNi_4B$ (*Cmcm*)*			
	B(2c)	B(2c)	B1(8f)	B2(4c)	B3(8f)	B4(4c)
Freq.(MHz)	-0.2331	-0.2433	0.2902	-0.1089	0.3537	-0.3841
η	0	0	0.9242	0.8992	0.6309	0.1596

*preliminary results.

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Anisotropy of magnetic fluctuations under pressures in ferromagnetic superconductor UGe_2

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Ferromagnetic (FM) superconductors have attracted much attention because of the superconducting (SC) state coexists with the FM state. Among them, UGe_2 has a unique phase diagram. The superconducting (SC) state in UGe_2 arises inside the FM state and is observed in the pressure range of P = 1 to 1.5 GPa [1]. The magnetization shows the enhancement at T_X in the FM phase [2]. The transition between FM1 with smaller ordered moment and FM2 with larger one is a broad crossover at ambient pressure. However, the crossover region terminates by applying the pressure. The terminal point is called a critical point (CP), above which the FM1-FM2 transition is of a first order. The CP in UGe_2 is reported as T_{CP} = 7 K and P_{CP} = 1.16 GPa. The FM1-FM2 transition disappears above P_X = 1.2 GPa where the superconducting transition temperature is highest. This suggests the SC is involved in the FM1-FM2 transition in UGe_2.

The nuclear magnetic resonance (NMR) measurements have been performed in UCoGe which is one of the ferromagnetic superconductors [3, 4]. The measurements of the spin-lattice relaxation rate $1/T_1$ in UCoGe indicate that UCoGe possesses the Ising type magnetic fluctuation along the magnetic easy axis (*c*-axis) [3]. In addition, it was reported that the anisotropic fluctuation correlates closely with the SC [4]. On the other hand, the details of the magnetic fluctuations in UGe_2 have not been investigated. In order to clarify the anisotropy of the magnetic fluctuations in UGe_2, we performed the ^{73}Ge nuclear quadrupole resonance (NQR) measurement under pressure.

We measured T_1 and the spin-spin relaxation time T_2 to clarify the anisotropy of the magnetic fluctuations near T_X. At $P < P_X$, we found that the magnetic fluctuation along the *a* axis at the boundary between FM1 and FM2 is enhanced toward CP. Figure 1 shows the temperature dependences of $1/T_1T$ and $1/T_2$ in the FM2 phase at P = 1.21 and 1.32 GPa($P > P_X$). $1/T_1T$ exhibits $T_1T \sim const.$ and has no anomaly. On the other hand, $1/T_2$ at both pressures shows complicated peak structure.

We will talk about the interpretation of the peaks of $1/T_2$. We also show the results of $1/T_1T$ and $1/T_2$ at P = 1.44 GPa.

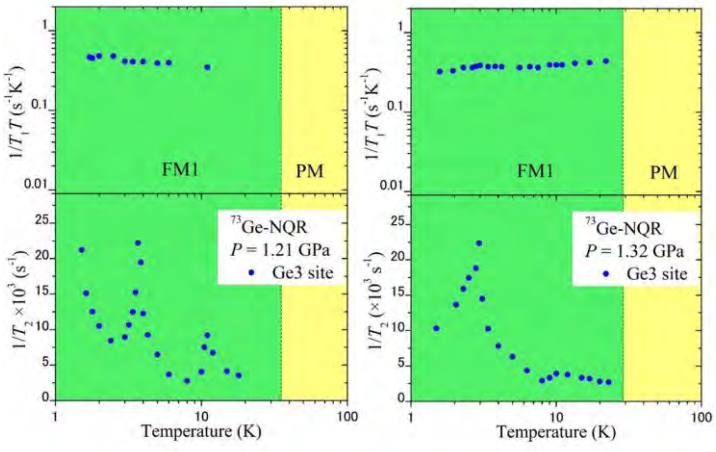

Figure 1. Temperature dependences of $1/T_1T$ and $1/T_2$ at P =1.21 and 1.32 GPa.

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Study of Single Crystal Growth and de Haas—van Alphen Effect in Thorium Compounds

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The 5*f*-electrons in a magnetic uranium compound possess dual nature: localized and itinerant features. Namely, the 5*f* electrons contribute to the volume of the Fermi surface and also to a magnetic moment at the uranium sites [1]. A non-5*f* thorium compound does not become a reference compound for the corresponding uranium compound because a valence of the Th atom with electron configuration $6d^2 7s^2$ are different from those of U^{3+} ($5f^3 6d^1 7s^2$) or U^{4+} ($5f^2 6d^2 7s^2$). The number of valence electrons in the thorium compound is, however, the same as that of a 4*f*-itinerant cerium compound. The topology of the Fermi surface in $ThIn_3$ [2] and $ThRu_2Si_2$ [3] is approximately the same as in 4*f*-itinerant $CeIn_3$ and $CeRu_2Si_2$, for example. The cyclotron effective masses are, however, significantly different between Th compound and Ce compound. Large cyclotron masses in Ce compounds are most likely due to the many-body quantum effects, such as the Kondo effect. To clarify the electronic states, the de Haas-van Alphen effect (dHvA) measurement and the energy band calculations play an important role in understanding the strongly correlated nature of *f*-electron systems.

Recently, we grew single crystal and clarified the Fermi surface and the cyclotron effective masses of $ThSb_2$, $ThBi_2$, and $ThCu_2Si_2$ by the dHvA measurement and the energy band calculations with shifted the 5*f*-partial density of states. In the present study, we have succeeded in growing single crystal of $ThAl_3$ with the hexagonal structure by Al-self-flux method for the first time, as shown in Fig. 1. The size of an obtained bar shape single crystal in $ThAl_3$ is about $1 \times 1 \times 5$ mm^3. We will present the results of the electrical resistivity, specific heat, and dHvA effect in the poster presentation.

Fig. 1. Single crystal ingots of $ThAl_3$.

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Heavy electronic states and spin splitting in $U_3Ni_3Sn_4$

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We have successfully grown a high quality single crystal of $U_3Ni_3Sn_4$ by the Bridgman method and explored its structural, magnetic and electronic properties by the means of single crystal diffraction, magnetization, heat capacity, electrical transport and de Haas-van Alphen (dHvA) effect [1]. The crystal structure and the bulk physical properties of single crystalline $U_3Ni_3Sn_4$ are in conformity with the previous reports [2-6]. Several closed Fermi surfaces with spherical topology are found in the angle dependence of the dHvA frequencies. Furthermore, the temperature dependence of amplitude of dHvA oscillation reveals the cyclotron effective masses up to $35m_0$. Local density approximation (LDA) band structure calculations considering U 5*f* electrons as itinerant gives 12 bands crossing the Fermi energy. The multitude of the Fermi surfaces comes from the splitting of the bands introduced by antisymmetric spin orbit interaction due to lack of an inversion centre in the crystal structure of $U_3Ni_3Sn_4$. This splitting is also observed experimentally in the frequency spectrum of the dHvA experiment in $U_3Ni_3Sn_4$, though the splitting energy is merely 23-24 K by using cyclotron effective mass and 68-100 K by using the band masses. These values are smaller than those observed in the *d*-electron systems, namely, 20-100 K in VSi_2, 200-300 K in $NbSi_2$ and 500-600 K in $TaSi_2$ [7]. Nevertheless, to the best of our knowledge, $U_3Ni_3Sn_4$ is the first non-centrosymmetric uranium system in which such a phenomenon has been observed. Our results suggest that the heavy electronic states strongly suppress the splitting energy in $U_3Ni_3Sn_4$. The field dependence of the amplitude of dHvA oscillations gives Dingle temperatures ~ 0.1 K, which corresponds to a mean free path of the conduction electrons up to 1950 Å.

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Electrochemical control of hysteretic current-voltage characteristics in single-crystal of Fe(Se,Te) superconductor

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The application of an electrochemical method to the iron chalcogenide superconductors has great potentials in enhancing their properties such as the superconducting transition temperature T_c. Actually, the increase of T_c was electrochemically accomplished by deintercalateing excess Fe [1], intercalating the spacer layers between FeX_4 (X=Se or Te) layers [2], or applying the strong electric field to an electric double layer [3]. However, this method has been limited to polycrystalline powders or thin film samples with large surface area, since the moving distance of ions in solids during electrochemical reactions is very short, thus requiring a large surface area per unit volume to obtain an effective change. Recently, we succeeded in applying the electrochemical method to monocrystalline $FeSe_{1-x}Te_x$ superconductors by combining it with the focused ion beam (FIB) microfabrication techniques [4]. This opens a new route to exploring the unique properties of the iron chalcogenide superconductors by using the electrochemical methods.

In this presentation, we report the electrochemical control of hysteretic current-voltage (I-V) characteristics in small bridge-type junctions of $FeSe_{1-x}Te_x$ superconductor, fabricated by using FIB techniques. In the previous study [5], we demonstrated that the c axis I-V curves mea $FeSe_{0.3}Te_{0.7}$ single crystal suggesting the formation of junctions (IJJs). However, in only FeX_4 layers, a question plays a role of barrier to for junctions (IJJs) still remains u the excess Fe mixing in the syr deintercaltation of the excess $FeSe_{1-x}Te_x$ crystals, as shown provide important information effects. We found out th electrochemical reaction tim hysteresis in the I-V curves an temperature [6]. This suggests observed even in pure FeSe excess Fe.

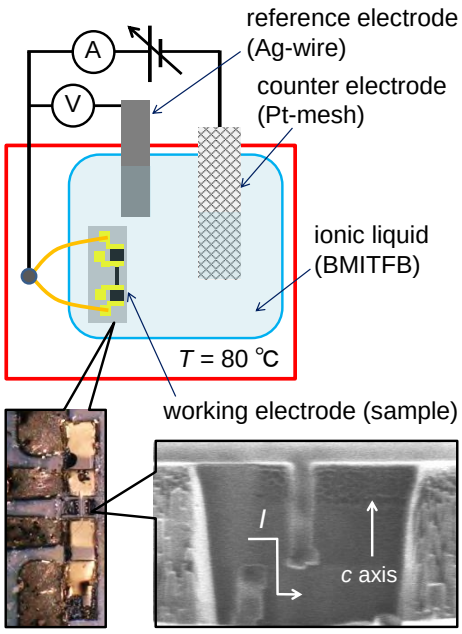

Fig. 1. Schematic of the electrochemical method applied to $FeSe_{1-x}Te_x$ crystals.

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Superconductivity in hexagonal BaPtAs and BaPtSb with an ordered honeycomb network

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Superconductors with honeycomb networks have attracted considerable interest since the theoretical predictions of exotic superconductivity in SrPtAs [1–3]. The compound SrPtAs exhibits superconductivity at 2.4 K [4], and crystallizes in the KZnAs-type structure ($P6_3/mmc$, D_{6h}^4, No. 194). The structure is globally centrosymmetric, although the spatial inversion symmetry is locally broken in the ordered PtAs honeycomb network. Possible superconducting states theoretically predicted for SrPtAs include a singlet-triplet mixed state [1], a chiral *d*-wave state [2], and an f-wave state [3]. These predictions have been examined experimentally. μSR measurements reported the breaking of time-reversal symmetry in the superconducting state, suggesting the chiral *d*-wave superconductivity as the most likely pairing state [5], whereas the NMR/NQR [6] and the magnetic penetration depth [7] measurements suggested a conventional s-wave pairing state. Another NQR measurement showed the absence of a Hebel–Slichter coherence peak and suggested two-gap superconductivity [8]. In order to settle this controversy, novel compounds with honeycomb networks should be developed and examined both experimentally and theoretically.

We report novel hexagonal structures of BaPtAs with ordered PtAs honeycomb networks, namely, SrPtSb- ($P\bar{6}m2$, D_{3h}^1, No. 187) and YPtAs-type ($P6_3/mmc$, D_{6h}^4, No. 194) structures [9]. Both structural phases exhibit superconductivity at 2.8 and 2.1–3.0 K, respectively [9]. In contrast, the previously known cubic LaIrSi-type ($P2_13$, T^4, No. 198) phase does not exhibit superconductivity above 0.1 K [9]. Moreover, we also report the emergence of superconductivity at 1.64 K in BaPtSb with the SrPtSb-type structure [10]. Spatial inversion symmetry is globally broken in the SrPtSb-type structure, whereas it is preserved in the YPtAs-type structutre. The discovery of superconductivity in these hexagonal platinum pnictides with PtPn (Pn = As, Sb) ordered honeycomb networks provides opportunities not only for the experimental examination of theoretically predicted chiral *d*-wave superconductivity but also for further theoretical studies on exotic states that result in the strong spin-orbit interaction of Pt under broken inversion symmetry.

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Superconductivity in trilayer $(PbSe)_n(TiSe2)_m$ misfit compound

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Misfit crystalline compounds are layered materials with two different crystal structure alternatively stacked along the *c*-axis. There are various compositions known, however, for the chalcogenides, the components are limited to the combination of monochalcogenide of Sn, Pb, Sn, Bi, and rare earth elements and dichalcogenides of Ti, V, Cr, Mo, W, Nb, and Ta [1].

Superconductivity is observed in mostly Nb and Ta compounds. It is also reported in Ti compound in $(PbSe)_{1.16}(TiSe_2)_2$ at the transition temperature (T_c) of 2.3 K [2]. This is similar to the superconductivity observed in intercalated $TiSe_2$ such as Cu_xTiSe_2 [3]. The similarities lie in their anisotropic nature and the relation with the charge density waves that disappears as the superconductivity comes in.

There are only mono- or bilayer TMD compounds reported in the single crystals of misfit crystalline compounds so far. We have synthesized trilayer-$TiSe_2$ compound, $(PbSe)_{1+\delta}(TiSe_2)_3$ for the first time and measured the superconductivity at 2.6 K as shown in Fig. 1. The crystal structure of stacking 3 $TiSe_2$ layers is confirmed by transmission electron microscopy as the conventional X-ray diffraction is not as powerful. The structure indicates the superconducting layer $TiSe_2$ as 3 layers compared to 2 layers, thus the anisotropy of superconducting state is expected to be modified. In the presentation, we would discuss the difference between bilayer and trilayer compounds.

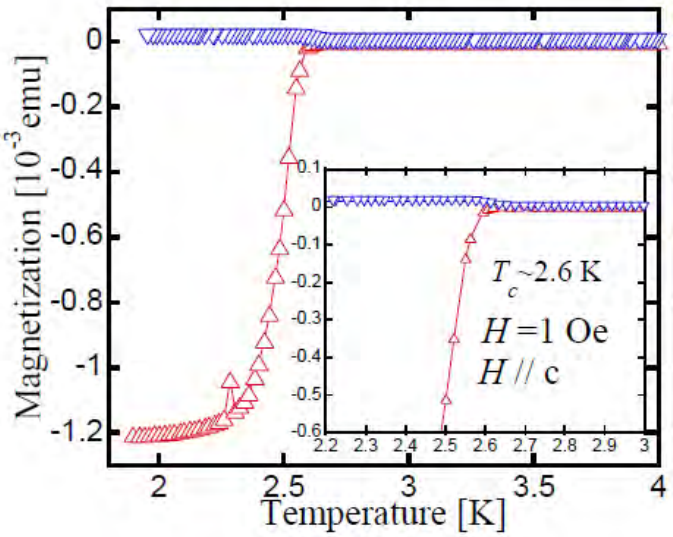

Fig. 1. Magnetization measurement on a single crystal of $(PbSe)_{1.16}(TiSe_2)_3$. The large diamagnetic signal shows the superconductivity below 2.6 K.

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Superconductivity in Laves structured Au compound

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Laves phase is one of the most profound structure to find superconductivity. There are several intermetallic materials to show superconductivity with various Laves structures [1]. Au_2Pb and Au_2Bi have the cubic Laves structure at the room temperature (T) and both show superconductivity below T_c = 1.2 K [2], and 1.8 K [3], respectively. The structural change at low T in Au_2Pb gives the material a very rich field to study [4-7].

We have synthesized the multicomponent alloy of $Au_2Bi_{1-x}Pb_x$ for x = 0-1 employing the high pressure synthesis method. The method allowed us to synthesize almost impurity-free compounds for the wide range of x. The obtained compounds showed superconductivity for all x associated with the enhanced T_c. The highest T_c is in the vicinity of x = 0.6 and is approaching to 3 K (Fig. 1). This drastic enhancement of T_c could be explained from the absence of density of states for the Au_2Pb and Au_2Bi while the strong spin-orbit coupling interaction for Bi and Pb as well as Au may play the important role.

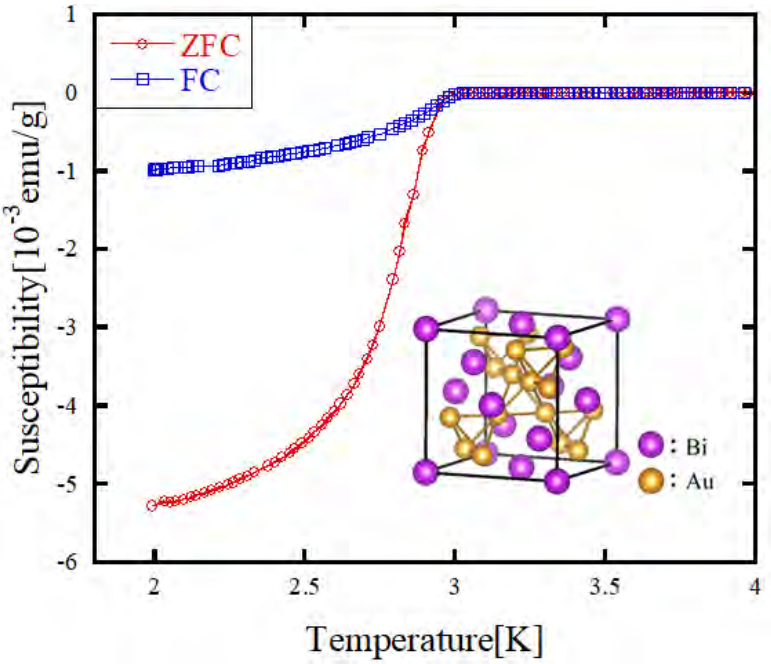

Fig. 1. Susceptibility in ZFC and FC for $Au_2Bi_{1-x}Pb_x$ (x = 0.6).

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Temperature dependence of the anisotropic displacement parameters U_{11} and U_{33} in $REO_{0.5}F_{0.5}BiS_2$ (RE = La, Ce and Pr)

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The layered bismuth chalcogenide ($BiCh_2$-based) superconductors discovered in 2012[1], are a new class of layered superconductor family but the pairing mechanisms of the superconductivity have not been understood. Theoretical calculations [2] and the angle-resolved photoemission spectroscopy (ARPES)[3] proposed unconventional pairing mechanisms in the $BiCh_2$-based superconductors. Furthermore, we showed the absence of selenium isotope effect on transition temperature in $LaO_{0.6}F_{0.4}Bi(S, Se)_2$, which may originate from non-phonon superconductivity mechanisms [4].

Since the $BiCh_2$-based system has a complicated layered structure, crystal structure analysis has important roles to understand the pairing mechanism of superconductivity in the $BiCh_2$-based systems. Particularly, anisotropic analysis of atomic displacement parameters is a powerful tool. As an important result, we showed a clear relationship between the emergence of bulk superconductivity and the suppression of the in-plane disorder in $REO_{0.5}F_{0.5}BiS_2$ (RE = La, Ce and Pr) [5].

In this study, we investigated the temperature dependence of the anisotropic displacement parameters for the $REO_{0.5}F_{0.5}BiS_2$. The in-plane displacement parameter U_{11} for the S1 site decreases with decreasing temperature from 600 to 300 K. However, below 300 K, U_{11} for the S1 site does not depend on temperature and saturates at around 0.09-0.04 Å^2. The fact that U_{11} for the S1 site does not depend on temperature may indicate that some local disorder or short-range structural distortion may be generated in the low temperature region.

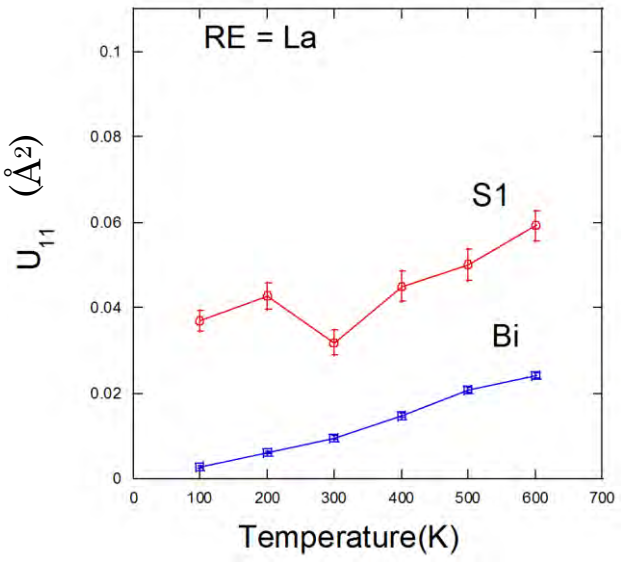

Fig. 1. Temperature dependence of the anisotropic atomic displacement parameter U11 for the s1 and Bi sites

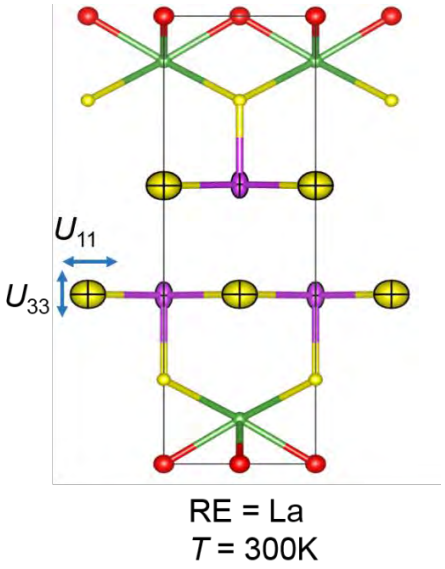

Fig. 2. Schematic model of the crystal structure of PrO0.5F0.5BiS2; 90%-probability displacement ellipsoids are outlined.

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^{75}As-NQR Investigation of Superconducting Phase in $Ru_{1-x}Rh_xAs$

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In 2012, Hirai et al. have reported that binary RuP and isostructural RuAs show metal-insulator transitions accompanied by structural transitions on polycrystalline samples [1]. In addition, they found that Rh-substitution for Ru suppresses the two transitions and then induces superconducting phase in both materials [1]. Inspired by their discovery, we have studied RuAs and $Ru_{1-x}Rh_xAs$ using nuclear quadrupole resonance (NQR) measurements.

In the metallic phase, RuAs crystalizes in the orthorhombic structure with *Pnma* space group. It is non-symmorphic structure composed of Ru zig-zag chain. The band calculations have suggested that the metallic phase possesses Fermi surface instability originating in the degenerated flat bands near the Fermi level. This degeneracy is protected by the non-symmorphic symmetry [2,3]. Recently we successfully obtained single crystal of RuAs by Bi-flux method, revealing clear successive metal-insulator transitions at T_{MI1} = 255 K and T_{MI2} = 190 K, compatible with the result for polycrystalline samples [3]. X ray diffraction measurement for the single crystal has revealed that the superlattice formation into monoclinic $P2_1/c$ space group in the ground state below T_{MI2}. A coupling between the modulated crystal structure and the calculated number of the *d* electrons at each Ru site proposes a formation of characteristic CDW. The phase transition at T_{MI2} is of first order, while the phase transition at T_{MI1} is accompanied by a strong divergence of the nuclear spin-lattice relaxation rate (Fig.1). This suggests that an instability of metal insulator transition in RuAs induces the strong critical fluctuations of some degree of freedom. The critical fluctuation is suppressed by the Rh substitution, and superconductivity with the maximum transition temperature is realized in the region where critical fluctuations are weakened significantly. Therefore, it is an intriguing hypothesis that superconductivity is mediated by the instability of the metal-insulator transition. As for RuP, ^{31}P-NMR measurement has shown a Hebel-Slichter peak below T_c, demonstrating that superconductivity is understood in the BCS framework [4]. It is still unclear whether the strong fluctuations observed at the ^{75}As nucleus in RuAs, which might be charge fluctuations, contribute the occurrence of superconductivity or not. We will discuss how superconductivity in $Ru_{1-x}Rh_xAs$ occurs near the phase boundary via ^{75}As-NQR measurements.

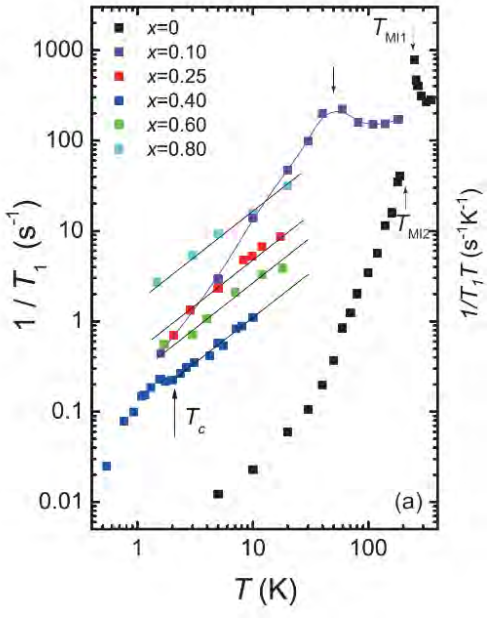

Fig. 1. Temperature dependence of $1/T_1$ for $Ru_{1-x}Rh_xAs$.

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Synthesis of BiS_2-based layered superconductors with high-entropy-alloy-type blocking layers

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Since the discovery of BiS_2-based layered superconductors in 2012, this family of compounds has received much attention as a new class of layered superconductors. The crystal structure composed of alternate stacks of electrically conducting BiS_2 layers and blocking layers is similar to that of the cuprate or Fe-based high-transition-temperature (T_c) superconductors. [1] The chemical pressure effect is essential for inducing superconductivity in $REO_{0.5}F_{0.5}BiS_2$ and can be systematically controlled by the alloying effect at the RE site of the blocking layer. The systematic shrinkage of the blocking layer was achieved by using smaller RE elements. When the chemical pressure is optimally applied, the in-plane Bi-S1 bond distance becomes short and bulk superconductivity is induced. [2] Furthermore, the in-plane chemical pressure effect suppresses in-plane local disorder at the S1 site, which is essential for the emergence of bulk superconductivity in this system.

In this study, we used the concept of high-entropy-alloy (HEA) for the RE site of $RO_{0.5}F_{0.5}BiS_2$. Samples with RE = $La_{0.3}Ce_{0.3}Pr_{0.2}Nd_{0.1}Sm_{0.1}$, $La_{0.2}Ce_{0.2}Pr_{0.2}Nd_{0.2}Sm_{0.2}$, $La_{0.1}Ce_{0.1}Pr_{0.3}Nd_{0.3}Sm_{0.2}$, and $La_{0.1}Ce_{0.1}Pr_{0.2}Nd_{0.3}Sm_{0.3}$ (See the left panel of Fig. 1) were newly synthesized in this study. (An HEA is defined as an alloy containing at least 5 elements with concentrations between 5 and 35 atomic percent, according to the paper by Yeh et al. [3]) Superconducting properties were investigated from resistivity and magnetization measurements.

Zero resistivity and clear diamagnetic susceptibility were observed for all the samples. The right panel of Fig. 1 shows that the plot of T_c as a function of lattice constant of *a* for the HEA-type samples located clearly higher temperature region than those of typical $REO_{0.5}F_{0.5}BiS_2$. This may indicate that the in-plane disorder is suppressed by the HEA effect, instead of lattice shrinkage (in-plane chemical pressure). [4]

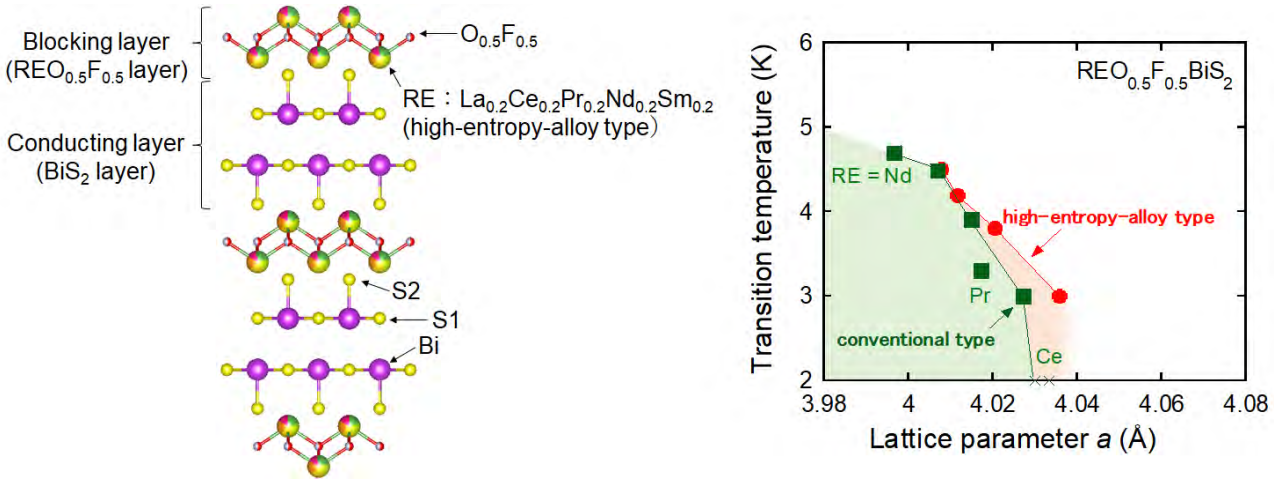

Fig. 1 (left) Crystal structure of HEA-type $REO_{0.5}F_{0.5}BiS_2$. (right) Superconductivity phase diagram of typical and HEA-type $REO_{0.5}F_{0.5}BiS_2$.

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Ultrasound attenuation around T_c of $Rh_{17}S_{15}$

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We present ultrasonic attenuation measurements in the vicinity of the superconducting transition temperature (T_C) of $Rh_{17}S_{15}$. The presence of strongly correlated superconductivity in $Rh_{17}S_{15}$ had a major impact on the condensed matter physics community. [1] Different from the *f*-electron systems, the formation of a heavy fermion (HF) state in *d*-electron systems is a rare event. Even in those cases, none of them exhibits superconductivity. $Rh_{17}S_{15}$, which is a 4*d*-electron compound is a HF superconductor with a relatively large electronic specific heat coefficient of γ = 104.8 mJ/K^2 mol and with a superconducting transition temperature of T_c = 5.4 K. [1-3] The superconductivity is considered to be arising from strong correlated charge carriers presumably due to the high density of states of *d* bands at the Fermi level. The crystal structure of $Rh_{17}S_{15}$ is described mainly on the basis of its belonging to cubic space group *Pm*3*m*. The structure contains 2 formula units with 64 atoms in the unit cell. There are four kinds of Rh and three different kinds of S atoms in the structure. The emphasis here is this crystal structure, i.e. the Rh(3*d*) has two Rh(6*e*) neighbors at 2.58 Å which is shorter than the nearest neighbor Rh-Rh distance (2.69 Å) in a cubic Rh sublattice. [1] This would result in narrow 4*d* band states in this system.

We performed ultrasound measurements on $Rh_{17}S_{15}$ as a function of temperature and magnetic field. The measurement was done by using a new designed experimental apparatus for the ultrasound measurement inserted into a commercially available physical property measurement system (PPMS). Figure 1 shows the low-temperature dependence of the shear elastic constant $c_E = (c_{11} - c_{12})/2$ exhibits strong softening from high temperature down to T_c, presumably due to the high density of states of *d* bands at the Fermi level. Figure 2 shows an overall view of the magnetic field dependence of the shear elastic constant c_E from -9 to 9 T. One can find a clear peak structure centered at 0 T appearing below T_c, reflecting the superconducting gap structure in $Rh_{17}S_{15}$. In this talk, we discuss the elastic property, and also the nature of the superconducting order parameter of $Rh_{17}S_{15}$.

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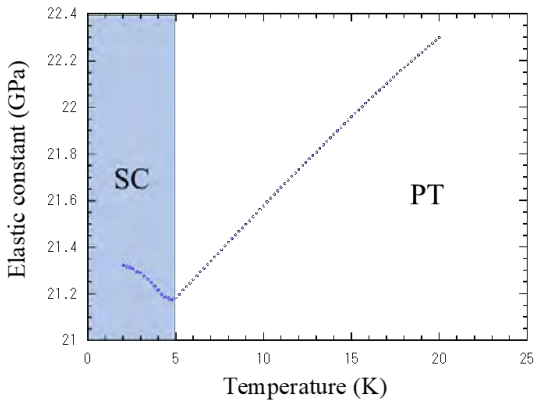

Fig. 1
Low-temperature dependence of c_E in $Rh_{17}S_{15}$.

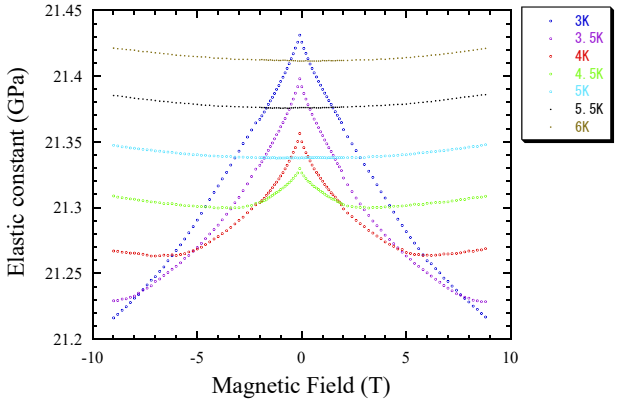

Fig. 2
Magnetic field dependence of c_E in $Rh_{17}S_{15}$.

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Theoretical Study on Quadrupole Fluctuation and Superconductivity in Fe-Based Superconductors.

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The rich variety of the phase diagrams in FeSe systems demonstrates the strong interplay between the nematicity, magnetism and superconductivity in Fe-based superconductors. Bulk FeSe emerges the tetragonal-orthorhombic structure (=electronic nematic) transition at T_s~90K and superconducting transition at T_c~9K, whereas the magnetic transition is absent [1]. In this superconducting state, strongly anisotropic gap functions are observed [2]. The relation between the nematicity and superconductivity is a significant unsolved problem. On the other hand, by introducing 10~15% electron carrier, the electronic nematic state is suppressed while T_c drastically increase to 60K. The fully-gapped s_{++} wave state without sign-reversing has been reported experimentally [3], and it cannot be explained by spin fluctuation theory using RPA and Migdal-Eliashberg approximation.

Here, we investigate the electronic state in FeSe systems focusing on the relation between the nematicity and superconductivity based on a multi-orbital Hubbard model by including both the spin-orbit interaction and the higher-order many-body effects called the vertex correction (VC). We find that, in bulk FeSe, the strong ferro-orbital fluctuations on *xz* and *yz* orbitals develop equally, and its divergence corresponds to the nematic transition [4]. The ferro-orbital order $n_{xz} \neq n_{yz}$ corresponds the ferro-quadrupole order $O_{x2-y2} \neq 0$. In the orthorhombic phase, however, the orbital fluctuation on the *yz* orbital becomes dominant, and the superconducting gap becomes large on the FSs with large *yz*-orbital component. The obtained orbital-selective gap structure is consistent with ARPES and QPI measurements [2]. In addition, we study the high-T_c state for electron-doped FeSe. We find that the moderate spin and quadrupole fluctuations develop due to the orbital-spin interplay through the VC. Then quadrupole fluctuations give rise to strong attractive pairing interaction since the electron-boson coupling constant is magnified by the VC. Because of the beyond Migdal-Eliashberg pairing mechanism, the fully-gapped s_{++} wave save is naturally obtained [5].

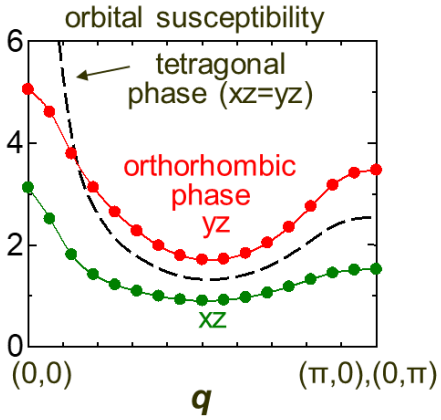

Fig. 1. Momentum dependence of orbital susceptibilities on xz and yz orbitals in orthorhombic phase. The dashed line shows the orbital susceptibility in tetragonal phase.

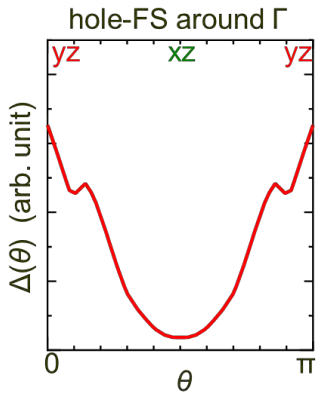

Fig. 2. Angle dependence of the gap function in orthorhombic phase.

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Nematic Quantum Critical Point in $FeSe_{1-x}S_x$ superconductors

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The electronic nematic states characterized by spontaneous rotational symmetry breaking have been intense debates because nematic fluctuations may also play a key role for superconducting-mechanism. Importance of nematic fluctuations has been suggested because various experiments reveal the nematic quantum critical point in optimally doped iron-based superconductors [1], however, nematic quantum criticality observed in these study is intertwined with antiferromagnetism, which causes difficultly to identify the essential effects of nematic fluctuations.

Iron-based superconductor FeSe is a key material to elucidate the role of nematic fluctuations due to the absence of magnetism at ambient pressure despite keeping high nematic transition temperature at $T_s \sim 90$ K [2]. Isovalent substitutions by S into Se sites effectively control the nematic transition temperature expected from chemical pressure effect without carrier doping. Nematic order completely disappears when the S substitution excceds 17 %. Suppression of nematic order in $FeSe_{1-x}S_x$ occurs without inducing the antiferromagnetic phase in contrast to high-pressure study [3]. This system is a promising candidate that may have a pure nematic quantum critical point without contamination from magnetism.

In order to clarify this putative nematic quantum criticality, we evaluate the nematic fluctuations in this system by elastoresistance measurements, which have been developed as sensitive probe of nematic fluctuations [4]. Elastoresistance is changes in resistance by applying strain, especially when strain works as conjugate field to nematic order, it linearly couple to nematic susceptibility. Our elastoresistance measurements reveal enhancement of nematic fluctuations towards nematic order explained by Curie-Weiss law and systematic changes against S substitution of both transition temperature and nematic-Weiss temperature that is bare nematic transition temperature in the limit of no electron-phonon coupling. This enhancement is still observed around $x \sim 0.17$ where nematic order is completely suppressed and nematic Weiss temperature changes its sign, suggesting the existence of the nematic quantum critical point [5]. $FeSe_{1-x}S_x$ provides an excellent platform to study the relationships between nematicity and superconductivity.

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Large magneto-optical Kerr effect and imaging of magnetic octupole domains in the antiferromagnetic Weyl metal Mn_3Sn

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When a polarized light beam is incident upon the surface of a magnetic material, the reflected light undergoes a polarization rotation. This magneto-optical Kerr effect (MOKE) has been intensively studied in a variety of ferro- and ferrimagnetic materials because it provides a powerful probe for electronic and magnetic properties as well as for various applications including magneto-optical recording. Recently, there has been a surge of interest in antiferromagnets (AFMs) as prospective spintronic materials for high-density and ultrafast memory devices, owing to their vanishingly small stray field and orders of magnitude faster spin dynamics compared to their ferromagnetic counterparts [1]. In fact, the MOKE has proven useful for the study and application of the antiferromagnetic (AF) state. Although limited to insulators, certain types of AFMs are known to exhibit a large MOKE, as they are weak ferromagnets due to canting of the otherwise collinear spin structure [2]. In the fully compensated collinear AFMs, where the MOKE is usually absent, quadratic magneto-optical effects such as the Voigt effect can be useful to determine the Néel vector [3]. On the other hand, recent theoretical and experimental progress has revealed that systems such as certain spin liquids and non-collinear AFMs can exhibit a large anomalous Hall effect (AHE) in zero applied magnetic field despite a vanishing magnetization [4,5]. Because the AHE has the same symmetry requirements as the MOKE, it is possible that the same class of AFMs may exhibit a Kerr rotation. Thus, the recent experimental discovery of a large AHE in the non-collinear AFM Mn_3Sn [5], which is recently reported to be a Weyl magnet [6], as well as its soft response to a magnetic field give promise for a potentially large MOKE character.

Here we report the first observation of a large MOKE signal in an AF metal at room temperature [7]. In particular, we find that despite a vanishingly small magnetization of $M \sim 0.002$ μ_B/Mn, the non-collinear AF metal Mn_3Sn exhibits a large zero-field MOKE with a polar Kerr rotation angle of 20 mdeg, comparable to ferromagnetic metals. Our first-principles calculations have clarified that ferroic ordering of magnetic octupoles in the non-collinear Néel state may cause a large MOKE even in its fully compensated AF state without spin magnetization. This large MOKE further allows imaging of the magnetic octupole domains and their reversal induced by magnetic fields. The observation of a large MOKE in an AF metal should open new avenues for the study of domain dynamics as well as topological AF spintronics.

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Charge disproportionation of Mn *3d* and O *2p* in $(LaMnO_3)_2(SrMnO_3)_2$ superlattices studied by a resonant x-ray scattering

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Orbital hybridization between metal and ligand ions plays a crucial role in the physical properties in the *d*- and *f*- electron system. Perovskite nickelate is a typical compound exhibiting the charge-transfer type metal-insulator transition [1]. The bandwidth dominates the localized and the itinerant character. There the strength of the orbital hybridization between Ni *3d* and O *2p* attributed to the Ni-O-Ni bond angle is directly connected with the bandwidth. Moreover, two kinds of charge orderings were proposed theoretically in the insulating phase [2]. In the case of the narrow bandwidth, the charge ordering occurs at the Ni site, $2Ni^{3+} \rightarrow Ni^{2+} + Ni^{4+}$. On the other hand, in the case of the wider bandwidth, all Ni ions are Ni^{3+}, while the oxygen sites show a charge disproportionation of the O *2p* electron. It indicates that the charge disproportionation of Ni *3d* and O *2p* is controlled by the degree of orbital hybridization between *3d* and *2p*, although such two kinds of charge orderings have never been clarified experimentally. The hybridized state of *3d* and *2p* becomes a hidden parameter in the insulating phase of RNiO$_3$.

Manganite superlattice $(LaMnO_3)_m(SrMnO_3)_n$ (L*m*S*n*) has widely been investigated as a stage to control Mn valence, since the Mn valences in the $LaMnO_3$ and the $SrMnO_3$ layers are 3+ and 4+, respectively [3]. Here we noted the charge disproportionation of Mn *3d* and O *2p*, which is expected to influence the conductivity properties through the orbital hybridization between Mn *3d* and O *2p*, as expected in RNiO$_3$. In order to elucidate the peculiar charge orderings, we have performed the resonant x-ray scattering (RXS) measurements in the L2S2 superlattices not only at the Mn $L_{2,3}$ edge but also at the O *K* edge, which can directly clarify the Mn *3d* and O *2p* electronic states, respectively. As a result, the large modulation of Mn *3d* electronic state was observed in the L2S2 superlattice, which shows a well insulating behavior. On the other hand, the charge disproportionation of O *2p* is much enhanced in the other L2S2 superlattice, of which the resistivity is smaller than that of the former. The oxygen magnetism reflecting the charge disproportionation of O *2p* was also revealed in the latter. It indicates that the charge disproportionation of the O *2p* reflects the strength of the *p-d* hybridization related to the conductivity in the superlattices. This study also points out that the RXS measurement is a key technique to evaluate an order parameter of the orbital hybridized state.

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Pressure Response of the Mixed Valence $RE_{2.75}C_{60}$ (RE: Sm, Eu) Fullerides Studied by Raman Spectroscopy

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Rare-earth (RE) fullerides constitute an intriguing class of highly-correlated molecular systems due to the strong coupling between two electronically active sublattices. Materials with composition $RE_{2.75}C_{60}$ exhibit mixed valence phenomena and undergo isosymmetric valence transitions under the influence of external stimuli such as temperature and pressure [1,2]. Pressure application on $Sm_{2.75}C_{60}$ causes a hysteretic lattice collapse at ~4 GPa accompanied by a colour change from black to golden [2], analogous to what is observed in Kondo insulators such as SmS and attributed to a Sm valence transition towards 3+ [3]. $Eu_{2.75}C_{60}$ exhibits a similar lattice response at ~4.5 GPa.

In this work, the high pressure response of $Sm_{2.75}C_{60}$ and $Eu_{2.75}C_{60}$ is probed by means of Raman spectroscopy. In $Sm_{2.75}C_{60}$, the well patterned spectrum profile disappears above 4 GPa, being indicative of the occurrence of an insulator-to-metal transition. The hysteretic restoration of the spectral profile upon pressure release is in excellent agreement with the high pressure XRD data [2]. On the other hand, the evolution of the Raman peaks in $Eu_{2.75}C_{60}$ can be followed after its lattice collapse. Remarkably, two peaks appear in the region of the breathing mode of C_{60} that – taking into account their frequency difference (~4 cm^{-1}), the similar pressure slopes of their frequencies and the pressure evolution of their relative intensities (Fig. 1) – can be assigned to Eu^{2+} and Eu^{3+}. The different pressure response of the Raman spectra of the two fullerides could be attributed either to the different origin of the mixed valence (valence fluctuations or spatial configuration of cations having different valence on different lattice sites) or to the different time scale of the valence fluctuations with respect to that of the Raman scattering.

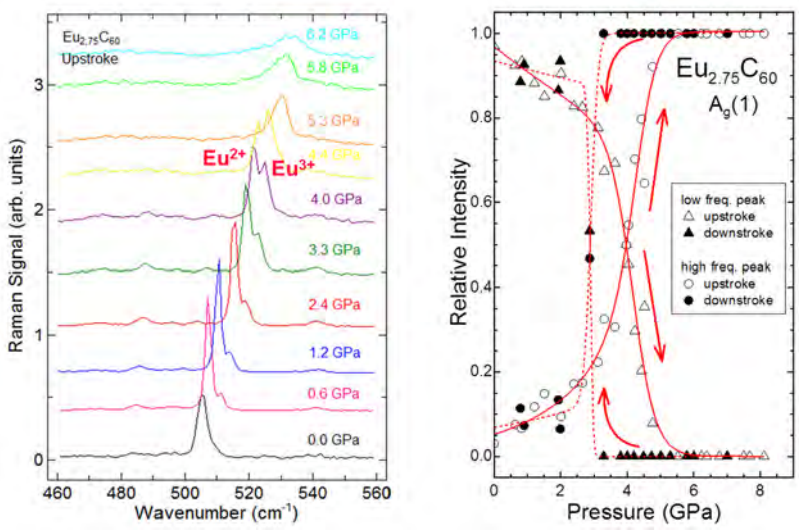

Fig. 1. Pressure evolution of the Raman data for $Eu_{2.75}C_{60}$.

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Magnetic phase diagram of $Sr_{2-x}La_xIrO_4$ synthesized by mechanical alloying

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Layered perovskite *5d* transition metal oxides Sr_2IrO_4 has attracted much attention because several experiments have revealed a novel spin-orbit-induced J_{eff}=1/2 Mott insulating behavior at low temperature. In this insulator with effectively one hole per Ir ion, this pseudospin remains a good quantum number and orders antiferromagnetically (T_N~240K). From the Monte Carlo study, Watanabe et al. point out that the superconducting state is found stable only by electron doping [1]. These results suggest that Sr_2IrO_4 is good candidate for unconventional superconductivity by carrier doping.

Experimentally, physical properties in electron doped Sr_2IrO_4 systems were extensively studied by several groups. Castaneda et al. reported the structure and magnetic properties of polycrystalline samples of $Sr_{2-x}La_xIrO_4$. They found that electrical resistivity increases with increasing La concentration and magnetic susceptibility results show the canted antiferromagnetism below 240K in both Sr_2IrO_4 and electron doped $Sr_{1.85}La_{0.15}IrO_4$ [2]. However, Neuron scattering and magnetic susceptibility measurements using single crystalline samples of $Sr_{2-x}La_xIrO_4$ revealed that long-range AF order was suppressed up to x = 0.04 and short-range AF order persisted up to x=0.12 by La doping [3]. T. F. Qi et al. reported oxygen vacancies into single crystal $Sr_2IrO_{4-\delta}$ ($0<\delta<0.04$) lead to significant reduction of resistivity and $Sr_2IrO_{4-\delta}$ (δ=0.04) shows metal-insulator transition at 105K [4]. Thus, the physical property differences between poly crystal and single crystal are still unsolved issue.

In this study, thus, we performed mechanical alloying (MA) synthesis because MA is well known to improve chemical reaction. We report the crystal structure and physical properties of $Sr_{2-x}La_xIrO_4$ using synchrotron powder x-ray diffraction, magnetic susceptibility, electrical resistivity and muon spin relaxation (μ SR) measurements.

The result of magnetic susceptibility in $Sr_{2-x}La_xIrO_4$ is shown in Fig. 1-(a). The observed values of magnetic susceptibility tend to decrease with La concentration. The La doping leads to significant straightening of the I-O-Ir bond angles, so the reduction of magnetic susceptibility is caused by not only the carrier doping but also the Ir-O-Ir bond angles. As for the T_N, a clear reduction of T_N is observed by La doping and T_N is changed from 240K (x=0) to 114K (x=0.13). These resistivity and magnetic susceptibility results are consistent with the previous results using single crystalline samples [3].

As for the zero field μ SR study, we found that short-range AF order is realized in $Sr_{1.9}La_{0.1}IrO_4$ and spin glass state is stabilized in low temperature region. The Ir moment estimated by the LF μ SR result is 0.09 μ_B, 4 times smaller than that of Sr_2IrO_4 (~0.4 μ_B). Furthermore, we found the relation between T_N and tetragonal distortion (c/a) in this system. This result suggests that magnetism of Sr214 system is strongly correlated with the crystal structure.

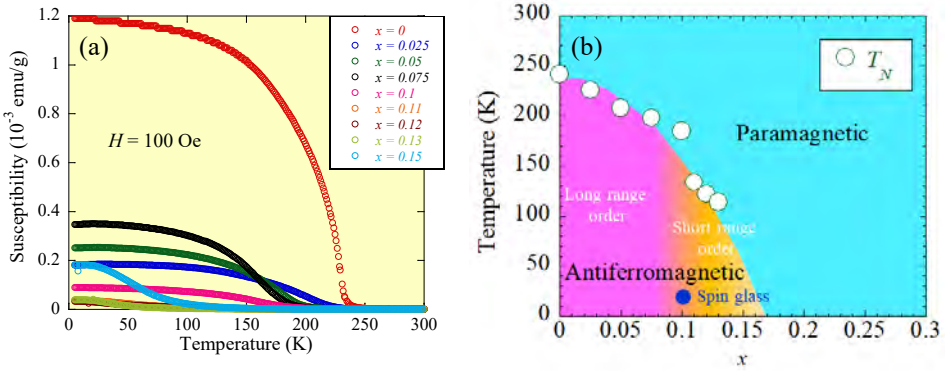

Figure 1 (a)Temperature dependence of magnetic susceptibility of $Sr_{2-x}La_xIrO_4$. (b) Magnetic phase diagram of $Sr_{2-x}La_xIrO_4$ determined by magnetic susceptibility and μ SR measurements.

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Thermodynamically stable magnetic skyrmion lattice at low temperatures in a polar magnetic semiconductor GaV_4Se_8

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In magnetic crystals without space-inversion symmetry, a uniform antisymmetric exchange interaction called the Dzyaloshinskii-Moriya interaction is allowed [1,2]. If the exchange interaction between two neighboring moments is ferromagnetic, the uniform antisymmetric interaction competes with the ferromagnetic exchange interaction, resulting in the formation of noncollinear magnetic structures such as magnetic skyrmions [3]. Magnetic skyrmions have been known to form a lattice structure in narrow temperature regions near the magnetic ordering temperatures in chiral crystals [4].

In this research, we established the magnetic field-temperature (*H*-*T*) phase diagram of a polar achiral lacunar spinel GaV_4Se_8 by means of ac magnetic susceptibility and magnetoelectric measurements on single crystals grown by chemical vapor transport method [5]. It undergoes the structural phase transition to a polar space group *R*3*m* at T_S=41 K, and magnetic phase transition at T_C=17.5 K. As the magnetic field increases, the magnetic state changes from cycloidal to skyrmion lattice and finally to forced ferromagnetic state. Both cycloidal and skyrmion-lattice magnetic orders induce electric polarization up to around 10 μC/m^2 compared with ferromagnetic order. In GaV_4Se_8, the skyrmion lattice phase seems to be stable down to 2 K (~0.1 T_C) while that in bulk chiral crystals have been observed down to about 0.9 T_C.

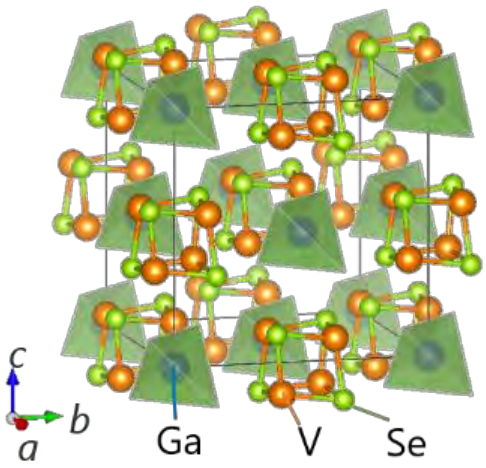

Fig. 1. Crystal structure of a lacunar spinel GaV_4Se_8 at room temperature with the cubic space group *F*-43*m*

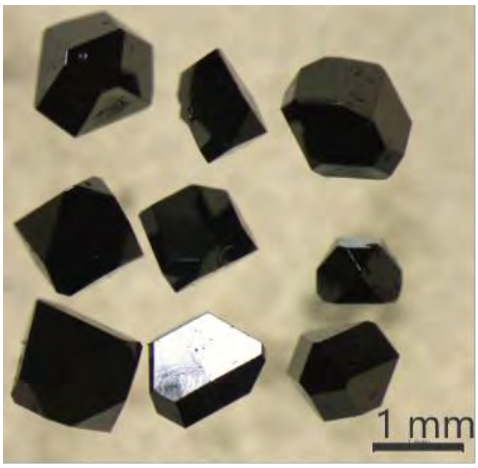

Fig. 2. Single crystals of GaV_4Se_8 grown by chemical vapor transport method

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Second Harmonic Generation of Noncentrosymmetric Antiferromagnet $BaMn_2As_2$

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$BaMn_2As_2$ has $ThCr_2Si_2$-type structure with the tetragonal space group $I4/mmm$, and shows G-type antiferromagnetic order below $T_N \sim 625$ K [1]. The magnetic structure breaks both spatial and time reversal symmetry, and the magnetic space group is $I4'/m'mm'$. Since the magnetic point group $4'/m'mm'$ is equivalent to the symmetry of the magnetic quadrupole (x^2-y^2 type), which is the second-rank magnetic multipole, $BaMn_2As_2$ can be recognized as a ferro-quadrupole magnet [2]. Insulators with the magnetic quadrupole order (e.g., Cr_2O_3) are known to show the linear magnetoelectric effect. Our interest is whether (semi-) conductors with the magnetic quadrupole order, which is the case of $BaMn_2As_2$, exhibit novel transport phenomena due to finite couplings between the conduction electrons and the magnetic quadrupole moments, just like an anomalous Hall effect in a ferromagnetic metal. However, the existence of magnetic domains makes it difficult to elucidate these phenomena. Therefore, in this study, we performed experiments of an optical second harmonic generation (SHG), which is a nonlinear optical response sensitive to the sample symmetry [3], to clarify the antiferromagnetic domain structure in $BaMn_2As_2$.

Single crystals of $BaMn_2As_2$ were synthesized by the self-flux method, and were characterized by the powder X-ray diffraction and the electrical conductivity measurements. In SHG measurements, the incident laser was irradiated onto the (001) surface at an incident angle of 45 degrees, and the reflected light with the twice energy was detected. As a result, we observed the characteristic polarization dependence of the SHG signal, which can be understood as interference between axial-i tensor and polar-c tensor contributions. By using this result, we succeeded in imaging antiferromagnetic domains (magnetic quadrupole domains) with the 0.1 - 1 mm scale.

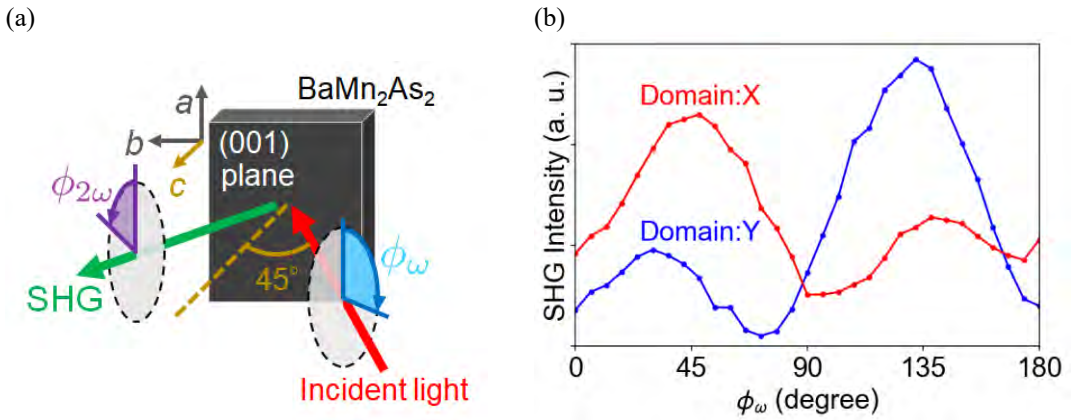

Fig. 1 (a) Experimental setup of SHG measurements. ϕ_ω and $\phi_{2\omega}$ are the polarization angle of the incident and reflected lasers, respectively. (b) Incident polarization angle (ϕ_ω) dependence of the reflected SHG intensity measured at $\phi_{2\omega} = 90°$. The red and blue line correspond to the experimental results for different antiferromagnetic domains.

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Giant negative magnetoresistance in antiferromagnet $BaMn_2Bi_2$

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ATM_2Pn_2 (A:alkaline-earth or alkali metal elements, TM:3d transition elements, Pn:pnictogen) compounds shows versatile physical properties such as unconventional superconductivity in K-doped $BaFe_2As_2$ (BFA). $BaMn_2Pn_2$ (BMPn, Pn:As, Sb, Bi) also belongs to this family and has been studied in analogy to BFA. BMPn, eing different from BFA, is a G-type antiferromagnetic (AF) semiconductor whereas BFA is a stripe-type AF semimetal. BMPn's do not show superconductivity, being in contrast to BFA.

Although superconductivity has not been observed in BMPn, other intriguing phenomena are reported. BMPn theoretically has an interesting magnetic ordering of hexadecapole, where the space inversion *P* and the time reversal *T* symmetry are broken, while the combination *PT* is preserved[1]. On the other hand, BMPn experimentally shows an anomalous magnetoresistance (MR) that depends drastically on the Pn substitution[2]. It suggests that the MR depends on such physical parameters as being changed by Pn substitution, for instance, strength of spin-orbit coupling (SOC), d-p hybridization between Mn 3d and Pn p orbitals. From these viewpoints, $BaMn_2Bi_2$ (BMB) can be expected to show the strongest SOC and hybridization considering the large atomic number and the p-orbital radius.

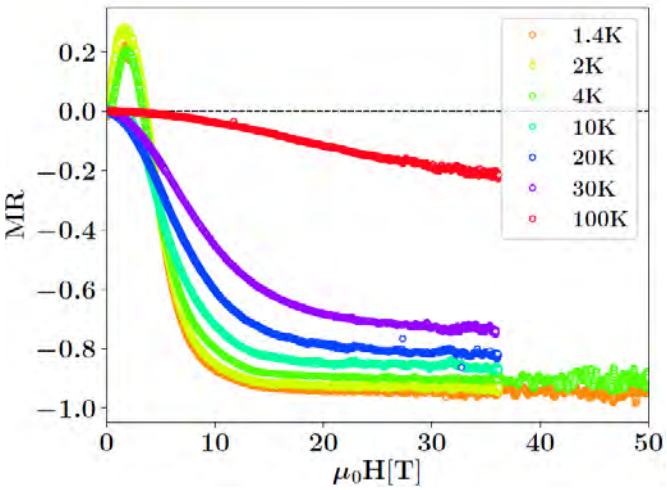

Fig.1: Magnetic field dependence of MR

According to this thought described earlier, we measure MR and Hall resistance (HR) of BMB as a function of temperature, magnetic field strength and its angle under the magnetic field (H) up to 9T using a Quantum Design Physical Property Measurement System (PPMS), for higher H of 18T employing the JASTEC 18T superconducting magnet at High Field Laboratory, Institution of Material Research, Tohoku, University, and H ≤ 55T with the 55T pulse magnet at the Center for Advanced High Magnetic Field Science, Osaka University. The magnetic field-strength dependence of longitudinal MR (LMR) is shown in Fig.1. At the high field and low temperature limit, LMR is intriguingly negative and becomes larger than 90%.

In this meeting, we report the details of anomalous MR observed in BMB, such as temperature dependence, and magnetic field strength- and angle- dependence. In addition, we also show other important physical properties i.e. Hall resistance, magnetic susceptibility, and specific heat. They indicate that BMB is a conventional antiferromagnetic semiconductor from these static properties. We will discuss the plausible interpretations on the anomalous MR.

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