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研究課題名(和文)原子レベルシミュレーションによる新奇六方晶機能製材料の設計

研究課題名(英文)Design of novel hexagonal functional materials by atomic level simulation

研究代表者

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研究成果の概要(和文):本プロジェクトは、デバイス応用をにらんで、大きな磁化と新奇な電気磁気相互作用を持つ六方晶YMnO3型または類似構造を持つ酸化物磁性体を探索した。具体的な成果は以下の通りである。 1 LuFeO3型システムにおいて、電場誘起スピン再配列と180°の電気磁気スイッチングを起こす、新しいコリニア型フェリ磁性を実現する方策を立案した。 2 (LuFeO3)m/(LuFe2O4)超格子の室温マルチフェロイック挙動の微視的なメカニズムを提案した。 3 .Co置換BiFeO3のスピン状態と強磁性発現の関係を提唱した。 4 . 斜方晶鉄酸化物、クロム酸化物におけるスピン再配列の微視的モデルを提唱した 5 . 室温極性金属を設計した。

研究成果の学術的意義や社会的意義

Our research provides a possible answer to the present quest for the multiferroic and Magnetoelectric system that can exhibit large magnetization and efficient magnetization control by the external means, for the potential application in novel devices such as voltage-controllable magnetic memories.

研究成果の概要(英文): The project aims to design magnetic materials with large magnetization and novel magnetoelectric (ME) coupling using computational simulations by exploring YMnO3 type hexagonal oxides and systems having related crystal structures. The findings are as follows; 1.An idea to realize novel non-collinear ferrimagnetic orders with potential electric field-controlled spin-reorientation (SR) transitions and 180° ME switching in LuFeO3 type systems (Under review, arXiv:2203.03841). 2.A probable microscopic mechanism to explain the RT multiferroic (MF) behavior of the (LuFeO3)m/(LuFe2O4)1 superlattices (Nat Commun 11, 5582 (2020)). 3.A predicted correlation between the spin-state and the MF properties of Co-doped BiFeO3 (Phys. Rev. Materials 6, 064401 (2022)). 4.Microscopic models of SR transitions in orthoferrites and orthochromites (Phys. Rev. Materials 5, 124416 (2021),Nat Commun 12, 1917 (2021)). 5. Design of prospective RT magnetic polar metals (Chem. Mater.33, 1594 (2021)).

研究分野: Condensed matter theory and materials physics

キーワード: Magnetoelectric effect Condensed matter theory Magnetism Spintronics Transition metal oxides

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本プロジェクトは、デバイス応用をにらんで、大きな磁化と新奇な電気磁気相互作用を持つ六方晶 YMnO3型または類似構造を持つ酸化物磁性体を探索した。具体的な成果は以下の通りである。 1. $LuFeO_3$ 型システムにおいて、電場誘起スピン再配列と 180°の電気磁気スイッチングを起こす、新しいコリニア型フェリ磁性を実現する方策を立案した。 2. $(LuFeO_3)_m/(LuFe_2O_4)$ 超格子の室温マルチフェロイック挙動($Nat\ Commun\ 11,5582\ (2020)$)の微視的なメカニズムを提案した。 3. Co 置換 $BiFeO_3$ のスピン状態と強磁性発現の関係を提唱した($Phys.\ Rev.\ Materials\ 6,064401\ (2022)$)。 4. 斜方晶鉄酸化物、クロム酸化物におけるスピン再配列の微視的モデルを提唱した($Phys.\ Rev.\ Materials\ 5,124416\ (2021),Nat\ Commun\ 12,1917\ (2021)$) 5. 室温極性金属を設計した($Chem.\ Mater.\ 33,1594\ (2021)$)。

1. Scientific background for the proposed research activity (研究開始当初の背景)

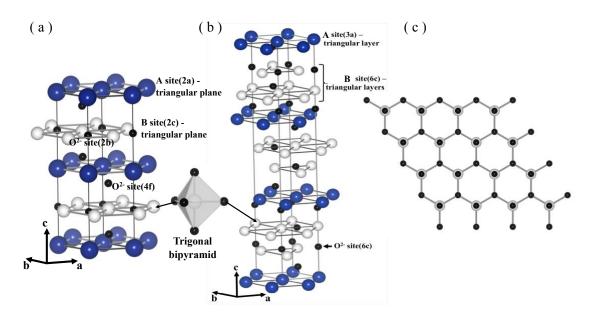


Figure 1 Undistorted high symmetry crystal structure of ABO₃($P6_3/mmc$) (a) and AB₂O₄($R\overline{3}m$) (b) transition metal oxides (A, B=cations). (c) Triangular arrangement of the B cations.

There has been considerable progress in the understanding of the microscopic mechanisms of the magnetoelectric (ME) coupling phenomenon which can enable the electric field control over magnetization (M). This topic of research is significant both from the fundamental and the applied physics points of view as large magnetization and strong ME coupling rarely coexist in a singlephase system at room temperature. The quest for effective microscopic mechanisms to realize this phenomenon is an active field of research. There has been increasing interest in the ABO₃ and AB₂O₄ (A, B = cations) transition metal (TM) oxides that crystallize in the hexagonal layered structures (see Figure 1) due to their potential to exhibit fascinating magnetic and electronic behavior, including room temperature multiferroic (MF) and ME behavior [Nature 537, 523 (2016)], topological orders [Nature 419, 818 (2002), Nature Mater 13, 163 (2014), Phys. Rev. Lett. 126, 157601 (2021), giant magnetic anisotropy [J. Phys. Soc. Jpn. 62, 1723 (1993), Phys. Rev. Lett. 103, 207202 (2009)] and spin-liquid behavior [Y. Shen et al., Nature 540, 559 (2016), Nat. Phys. 15, 262 (2019)], thereby offering sufficient scope for designing potential materials with fascinating properties. As illustrated in Figure 1, the B-site cation is surrounded by a trigonal bipyramid arrangement of oxygen atoms and in the planes of the corner-sharing trigonal bipyramids the B cations form triangular lattice. These planes are layered with the triangular planes formed by the A-site cations. A common feature of these materials is that the spins are antiferromagnetically coupled in the triangular lattice (see Figure 1(c)) and hence, are **geometrically frustrated**. Also, the ABO₃ systems (R = Sc, Y, In, Dy-Lu and B = Mn, Fe) exhibit ferroelectric behavior well above room temperature [Acta Crystallographica16, 957 (1963)], which is driven by the buckling of the BO₅ bipyramids and a subsequent trimerization of the Asite ions [Nature Materials 3, 164 (2004), Phys. Rev. B 72, 100103 (2005)]. A ME coupling mechanism which can lead to the 180° ME switching phenomena and the formation of topologically protected ME domain structures was predicted in LuFeO₃[Nat Commun 5, 2998 (2014)]. In addition to the structural complexity, various other factors contribute to dictate the electronic and magnetic behavior of these frustrated magnets, such as charge ordering, spin-orbit coupling and inter-triangular layer magnetic interactions. The challenge, therefore, is to develop material-property guidelines to tailor and predict the properties of these materials. In particular, the bearing of the atomic order or disorder on the functional properties of these materials is least explored, which was the main objective of this proposed research activity. Further in depth understanding of the ferroelectricity and it's coupling with magnetism within this hexagonal and related frame of lattice would guide researchers to design new materials with novel magnetic and ME phenomena with potential memory applications.

A polar Fe⁺²/Fe⁺³ charge ordered state was reported to induce electric polarization (*P*) in LuFe₂O₄[Nature 436, 1136 (2005)] and this finding initiated huge research activity. However, recent studies find that the ground state structure of LuFe₂O₄ is rather an antiferroelectric charge ordered phase [Nature 537, 523 (2016)]. On the other hand, LuFeCoO₄ exhibits relaxor ferroelectric behavior [J. Phys.: Conf. Ser. 320, 012084 (2011)]. Despite a large number of studies, ferroelectric behavior of these systems is far from understood. Recently, strong ferroelectric distortions have been observed in the LuFe₂O₄ layer [Nature 537, 523527 (2016)] induced by the robust geometric ferroelectric LuFeO₃ in (LuFeO₃)_m/(LuFe₂O₄)₁ superlattices. (LuFeO₃)_m/(LuFe₂O₄)₁ superlattices have been reported to show switching of the direction of *M* with the reversal of the direction of *P*. However, the mechanism that can lead to such coupling between the collinear ferrimagnetic *M* reported for these superlattices and FE *P* that can lead to 180° switching phenomena in these superlattices is not understood yet.

2. **Purpose of the research project: (**研究の目的)The objectives of the proposed research program are,

I. To study the electronic and magnetic behavior of the hexagonal ferrites in the limit of strong magnetic anisotropy and Dzyaloshinskii-Moriya (DM) coupling. LuFe₂O₄ exhibits

giant magnetic anisotropy, primarily originating from the degenerate $3d_{xz}$ electronic state of the Fe⁺² ion under a trigonal bipyramid oxygen environment (associated Fe-3*d* level splitting is schematically presented in Figure 2). The magnetic and electronic properties of LuFe₂O₄ having equal concentrations of Fe⁺² and Fe⁺³ ions are well explored [*Nature* 537, 523 (2016)]. In the present study we have explored the effect of the formation of the Fe²⁺/Fe³⁺ ordered structures in the magnetic and ME properties of the LuFeO₃ and (LuFeO₃)_m/(LuFe₂O₄)₁ superlattices. While in the former system the charge-ordered (CO) state can be formed due to the electron doping (by appropriate cation/anion substitutions), in the latter this phenomenon was controlled by the specific layering of the superlattices.

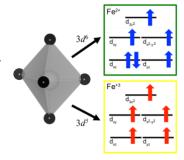


Figure 2The crystal filed splitting of the 3*d* states of Fe under the trigonal bipyramid oxygen environment.

II. To explore the stability of competing magnetic phases and spin-reorientation transition phenomena. Formation of multiple magnetic sublattices and strong interaction between them lead to the formation multiple magnetic phases and transitions like spin-reorientation (SR) transitions between them. The SR phenomenon has been observed in many ABO₃ type perovskite oxides systems. However, the underlying microscopic origin of this phenomenon using a material specific theoretical approach is less explored. In the present research activity, we have explored the microscopic origin of SR transitions considering both hexagonal and perovskite phases of ABO₃ oxides. We have also aimed is to develop mechanisms that lead to the efficient control over the SR transitions by the external means, such as electric field and optical stimuli [Nat. Mater. 20, 607-611 (2021)].

III. To understand and predict the electronic and magnetic behavior of the binary $A(BB')O_4$ systems (where B, B' = 3d TM ions) as a function of TM d-level occupancy. While the hexagonal phase has been synthesized for numerous 3d-3d transition metal combinations [Progress in Solid State Chemistry 43, 37 (2015)], the electronic and magnetic properties of these materials are less explored. One of the most studied materials of this family is LuFe₂O₄, which is a robust insulator with a large band gap [Phys. Rev. Lett. 101, 227602 (2008)]. In the proposed research efforts, we have investigated and attempted to predict the relation between crystal structure and the functional properties of the LuB_xB'_{1-x}O₄ systems through detailed investigation of the structural, electronic and magnetic phase stabilities as functions of the TM 3d-level occupancy.

3. Research method (研究の方法)

Ground state calculations (Density Functional Theory (DFT)): We used a combination of theoretical tools, such as DFT based electronic structure calculations, group theory, microscopic models and finite temperature Monte Carlo simulations to achieve our research goals. We conducted various levels of DFT calculations, such as energies of various structural and magnetic phases, equilibrium crystal structures, phonon dispersions, dielectric properties and electric polarization using Berry phase method, which is the most computationally heavy component of the present research activity. In order to conduct DFT calculations, we currently have two computational facilities, (1) a group private computer cluster and (2) access to Tokyo Tech supercomputer TSUBAME. The group also has the licensed access to DFT based Fortran code VASP and Wien2k.The cation ordered configurations were determined by using CASM (https://prisms-center.github.io/CASMcode_docs/) and the cation disordered phases were modeled by creating the special quasi-random structures (SQS) (ATAT).

Spin models to study the magnetic properties at finite temperature: In these frustrated magnetic systems, the relevant magnetic interactions are between TM magnetic moments and can be described through a Heisenberg spin model Hamiltonian, $H = \sum_{i,j} J_{ij} \vec{S}_i \cdot \vec{S}_j + \sum_{i,j} \vec{D}_{ij} \cdot \vec{S}_i \times \vec{S}_j + \sum_i \vec{S}_i \cdot \hat{\tau}_i \cdot \vec{S}_i$, where J_{ij} represents the symmetric isotropic exchange interactions, \vec{D}_{ij} represents the DM interactions and $\hat{\tau}_i$ is the single-ion anisotropy. The relevant interactions were considered through group theoretic symmetry analysis. The values of the magnetic interactions were estimated by performing total energy calculations for finite number of collinear and non-collinear spin structures. Suchan approach not only explains ground state spin structure, but also can be used for finite temperature analysis through Monte Carlo (MC) simulations [Nat Commun5, 2998 (2014), Nature 537, 523527 (2016)].

4. Research results (研究成果)

Designed non-collinear ferrimagnetism and its coupling with the ferroelectric order in LuFeO₃ (Under review, arXiv:2203.03841): Here, we have endeavored to design hitherto unobserved non-collinear ferrimagnetic orders characterized by high *M* and have coupled them with an improper ferroelectric (FE) order in the hexagonal LuFeO₃ that exhibits interesting

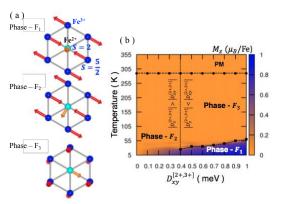


Figure 3 (a) Identified non-collinear ferrimagnetic orders F_1 , F_2 and F_3 . Red and orange arrows represent Fe^{3+} and Fe^{2+} spins, respectively. (b) Observed stable magnetic phases as a function of temperature and inter-sublattice DM interactions $(D_{xy}^{[2+,3+]})$.

topological orders. In our proposed model, the DM interactions between the magnetic ions and their coupling with the FE order is at the root of these magnetic and magnetoelectric (ME) phenomena. The proposed two-sublattice magnetic system, generated by a specific Fe²⁺/Fe³⁺charge-ordered (CO) state, forms multiple energetically close, non-collinear ferrimagnetic orders, thereby enabling the manipulation of the microscopic magnetic interactions and the triggering of SR transitions by various efficient means. The two-sublattice structure was realized in the hexagonal phase of LuFeO₃ doped with electrons. This electron doped system is characterized by $P \sim 15 \mu C/\text{cm}^2$, $M \sim 1.1 \ \mu_B/\text{Fe}$ and magnetic transition near room temperature (~ 290 K). Based on the coupling between the magnetic interactions and the FE primary order parameter observed in this system, microscopic mechanisms to achieve electric field

E induced SR transitions and 180° switching of the direction of M are proposed.

Predicted charge and ferrimagnetic order in (LuFeO₃)_m/(LuFe₂O₄)₁ MF and ME superlattices (Nat Commun 11, 5582 (2020)): In LuFeO₃, an improper FE behavior with an electric polarization of $P \sim 6.5 \ \mu C/\text{cm}^2 \text{ below} \sim 1040 \text{ K}$ and canted antiferromagnetic (AFM) order with induced $M \sim 0.03 \ \mu_B/\text{Fe}$ below $\sim 147 \ \text{K}$ were reported. On the other hand, LuFe₂O₄ exhibits a coupling between charge and magnetic order which leads to the formation of collinear ferrimagnetic behavior with considerably high $M \sim 0.8-1.4 \mu_B/\text{Fe}$ below ~ 240 K. Atomically engineered superlattices of LuFeO₃ and LuFe₂O₄ reportedly exhibited near room temperature MF and ME behavior [Nature 537, 523 (2016)]. Both the magnetic transitional temperature and M were found to be enhanced in these superlattices. Employing DFT calculations and finite temperature MC simulations, we showed that with an increase in the thickness of the FE LuFeO₃ layer there was a reduction in the magnetic frustration in the ferrimagnetic LuFe₂O₄ layer and a subsequent rise in the magnetic transition temperature. Moreover, we showed that the formation hole doped and Fe²⁺/Fe³⁺ CO non-polar ferrimagnetic layer can contribute to enhance the magnitude of **M**. A comparative analysis of the experimentally observed and calculated Magnetic circular dichroism (MCD) spectra furnished further evidences in support of this theoretical prediction.

Proposed microscopic mechanism of SR transitions in various perovskite phase of ABO₃ transition metal oxides (*Phys. Rev. Materials 5, 124416 (2021), Nat Commun 12, 1917 (2021)*): Spin reorientation (SR) transitions and other related magnetic phenomena, originating out of the

complex interplay between multiple magnetic sublattices, are scientifically interesting and have a wide variety of commercial applications. By means of DFT calculations and finite temperature MC simulations, we explored the possible origins of SR transition of Cr spins in NdCrO₃. We show that at the root of the observed SR transition in NdCrO₃, is a delicate balance between Nd-Cr magnetic isotropic exchange interactions, single ion anisotropy of Nd and Cr ions. As shown in Figure 4, the G_v - G_z SR transition strongly depends on the relative strength of Nd-Cr isotropic exchange with respect to Cr-Cr interaction γ interactions. Our results also propose a hitherto unobserved collective magnetic

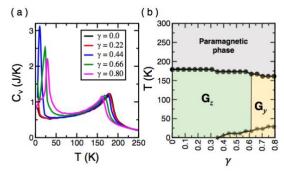


Figure 4 (a) calculated temperature dependence of specific heat for a choice of γ values. The second peak represents SR transition. (b) Magnetic phase diagram in T- γ plane. G_z and G_y represent G-type AFM order in Cr sublattice with spins orientated along z and y axes, respectively.

ordering in Nd sublattice. The detection of this ordering is, however, difficult as it is an extreme low temperature phenomenon. Therefore, further investigations are required before anything conclusive is said in this regard.

Recently, a non-trivial Pb²⁺/Pb⁴⁺ CO state and a SR transition from a canted AFM order with Fe spins oriented along the crystallographic a-axis (G_a) to a collinear AFM structure with spin moments along the b-axis (G_b) near 418 K was observed in PbFeO₃. We showed that the peculiar arrangement of the Pb ions leads to the creation of the two magnetic Fe1 and Fe2 sublattices with mutually competing magnetic anisotropy energies. While the former energetically favors the orientation of the spins along the b axis, the latter, in contrast, favors the a-axis spin orientation. At high temperatures, it is this which is expected to contribute to drive the SR transition. Our work is expected to introduce a unique opportunity of inducing magnetic phase transition ($M = 0 \leftrightarrow M \neq 0$) by driving a redistribution of Pb ions via an external electric E field and/or strain.

Other relevant research results funded by the present project (* corresponding author):

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5 . 主な発表論文等

「雑誌論文〕 計9件(うち査読付論文 9件/うち国際共著 9件/うちオープンアクセス 2件)

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1.著者名	4.巻
Fan Shiyu、Das Hena、Rebola Alejandro、Smith Kevin A.、Mundy Julia、Brooks Charles、Holtz Megan	11
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Site-specific spectroscopic measurement of spin and charge in (LuFe03)m/(LuFe204)1 multiferroic superlattices	2020年
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Nature Communications	5582
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10.1038/s41467-020-19285-9	有
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掲載論文のDOI(デジタルオブジェクト識別子)	査読の有無
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掲載論文のDOI (デジタルオブジェクト識別子)	査読の有無
10.1021/acs.chemmater.0c02976	有
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3.雑誌名 Chemistry of Materials	6.最初と最後の頁 4748-4758
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1.著者名 Kei Shigematsu, Keisuke Shimizu, Kazumasa Yamamoto, Takumi Nishikubo, Yuki Sakai, Sergey A. Nikolaev, Hena Das, and Masaki Azuma	4.巻
2 . 論文標題 Strain Manipulation of Magnetic Anisotropy in Room-Temperature Ferrimagnetic Quadruple Perovskite CeCu3Mn4012	5.発行年 2019年
3.雑誌名 ACS Appl. Electron. Mater.	6.最初と最後の頁 2514-2521
掲載論文のDOI(デジタルオブジェクト識別子) 10.1021/acsaeIm.9b00547	 査読の有無 有
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2.論文標題	5 . 発行年
Exploring the correlation between the spin-state configuration and the magnetic order in Co-	2022年
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3.雑誌名	6.最初と最後の頁
Physical Review Materials	64401
掲載論文のDOI(デジタルオブジェクト識別子)	査読の有無
10.1103/PhysRevMaterials.6.064401	有
オープンアクセス	国際共著
オープンアクセスではない、又はオープンアクセスが困難	該当する

〔学会発表〕 計6件(うち招待講演 2件/うち国際学会 4件)

1.発表者名

Hena Das

2 . 発表標題

Microscopic origin of near room-temperature multiferroic phenomena in (LuFeO3)m/(LuFe2O4)1 superlattices

3 . 学会等名

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4.発表年

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1.発表者名

Hena Das

2 . 発表標題

Unravelling near room temperature multiferroic phenomena in the hole doped LuFe204 based superlattices

3.学会等名

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4 . 発表年

2019年

1.発表者名

Hena Das

2 . 発表標題

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3 . 学会等名

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4.発表年

2019年~2020年

1 . 発表者名 若崎翔吾,Hena Das,山本樹,酒井雄樹,西久保匠,東正樹,町田晃彦,綿貫徹	
2.発表標題	
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3.学会等名	
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1 . 発表者名 大橋 孔太郎,山本 一理,重松 圭,Hena Das,東 正樹

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3 . 学会等名

2019年

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4 . 発表年 2019年

1.発表者名

若崎翔吾,重松圭,山本隆文,Hena Das,東正樹,Guowei Zhao,鈴木耕太,菅野了次,Randy Jalem,館山佳尚

2 . 発表標題

新規Li イオン伝導体Li40(Br,F)2 の合成及び構造解析

3 . 学会等名

日本セラミックス協会2020年年会(国際学会)

4.発表年

2019年~2020年

〔図書〕 計0件

〔産業財産権〕

〔その他〕

6.研究組織

Ο,			
	氏名 (ローマ字氏名) (研究者番号)	所属研究機関・部局・職 (機関番号)	備考

7. 科研費を使用して開催した国際研究集会

〔国際研究集会〕 計0件

8. 本研究に関連して実施した国際共同研究の実施状況

共同研究相手国	相手方研究機関
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