Abstract book
of
Spintronics and Core-to-Core Workshop 2017

Date: March 20-22, 2017
Place: Serni Hankyu Hotel, Osaka, Japan

About the Workshop

Purpose of the workshop:
The purpose of this workshop is to report and discuss the recent results on Spintronics research organized by Center for Spintronics Research Network (CSRN) in 2016FY and on Computational Nano-Materials Design on Green Energy organized by JSPS Core-to-Core Program in 2016FY. Based on the reports and discussions in the workshop, we will create the new concepts and proposals for the future collaborations related to the computational materials design and realization of energy-saving, energy-creation materials, and devices, such as spintronics, permanent magnets, moltronics, quantronics, thermoelectric power, superconductivity and topotronics. Based on the discussions, we will summarize the collaborative researches and propose a new proposal for the future collaborations.

Organizers and committee:

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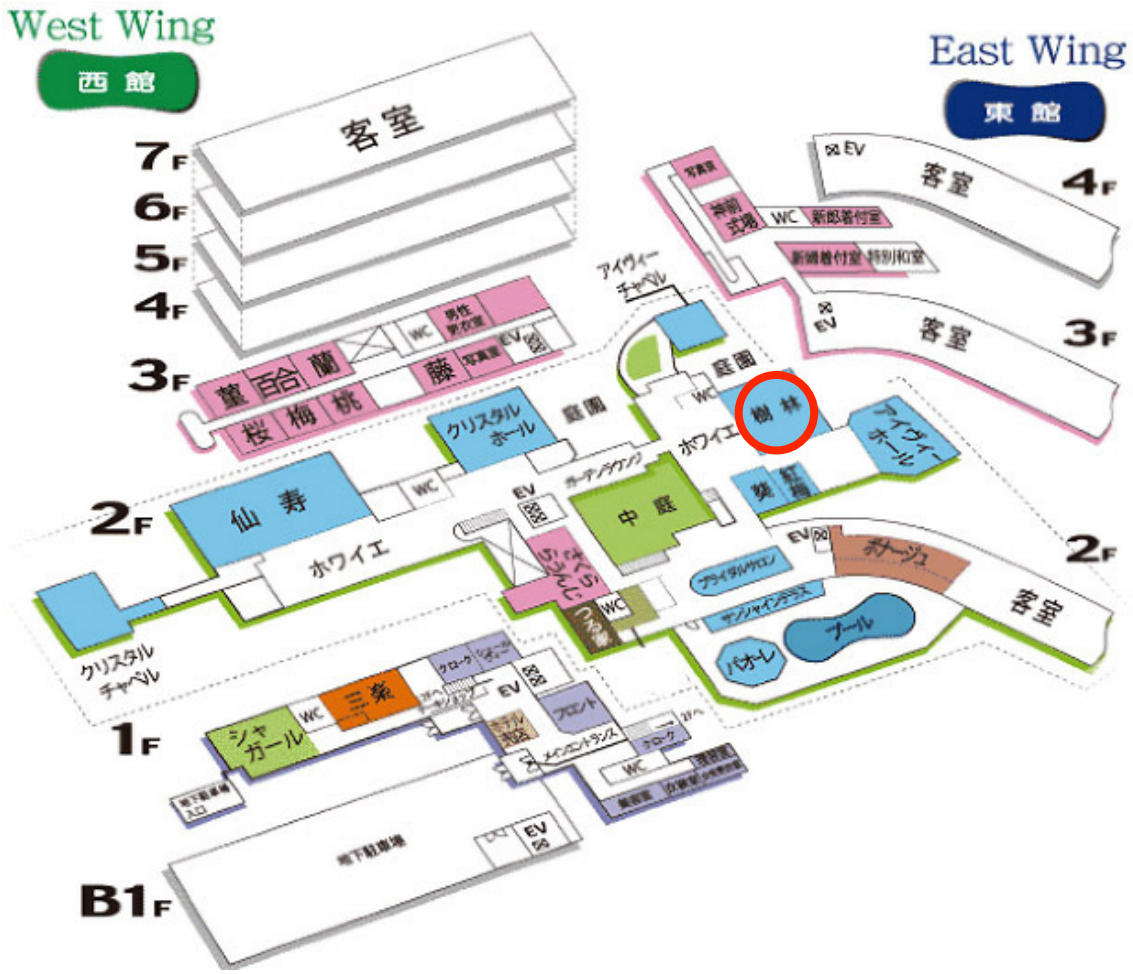
Sponsors:

- Center for Spintronics Research Network (Osaka University, The Univeristy of Tokyo, Tohoku University, and Keio University).
- JSPS Core-to-Core Program on “Computational Nano-materials Design on Green Energy”.
- International Joint Research Promotion Program, Osaka University (Japan-Austria, and Japan-Sweden).

Workshop information

Venue:
Senri Hankyu Hotel: Shinsenri-Higashimachi 2-1, Toyonakashi, Osaka, Japan.
(tel +81-6-6872-2211)
The workshop will be held at Room *Julin* (樹林), which is located on the second floor (2F) at East Building in Senri Hankyu Hotel.



Access:
The Senri Hankyu Hotel is located near the Osaka Monorail station of Senri-Chuo, Toyonaka, Osaka. You will be able to come there using the Osaka Monorail line from Itami Airport or from Hankyu Hotarugaike station. Persons arrived at Kansai airport will be come there using a shuttle bus from the airport to Hotarugaike.

Presentation regulation:
English is used in all the presentations. Speakers from abroad and introduction talks: 20 minutes (15 minutes for talk, 5 minutes for discussion). Domestic speakers: 15 minutes (10 minutes for talk, 5 minutes for discussion). However, the posters were described in Japanese.

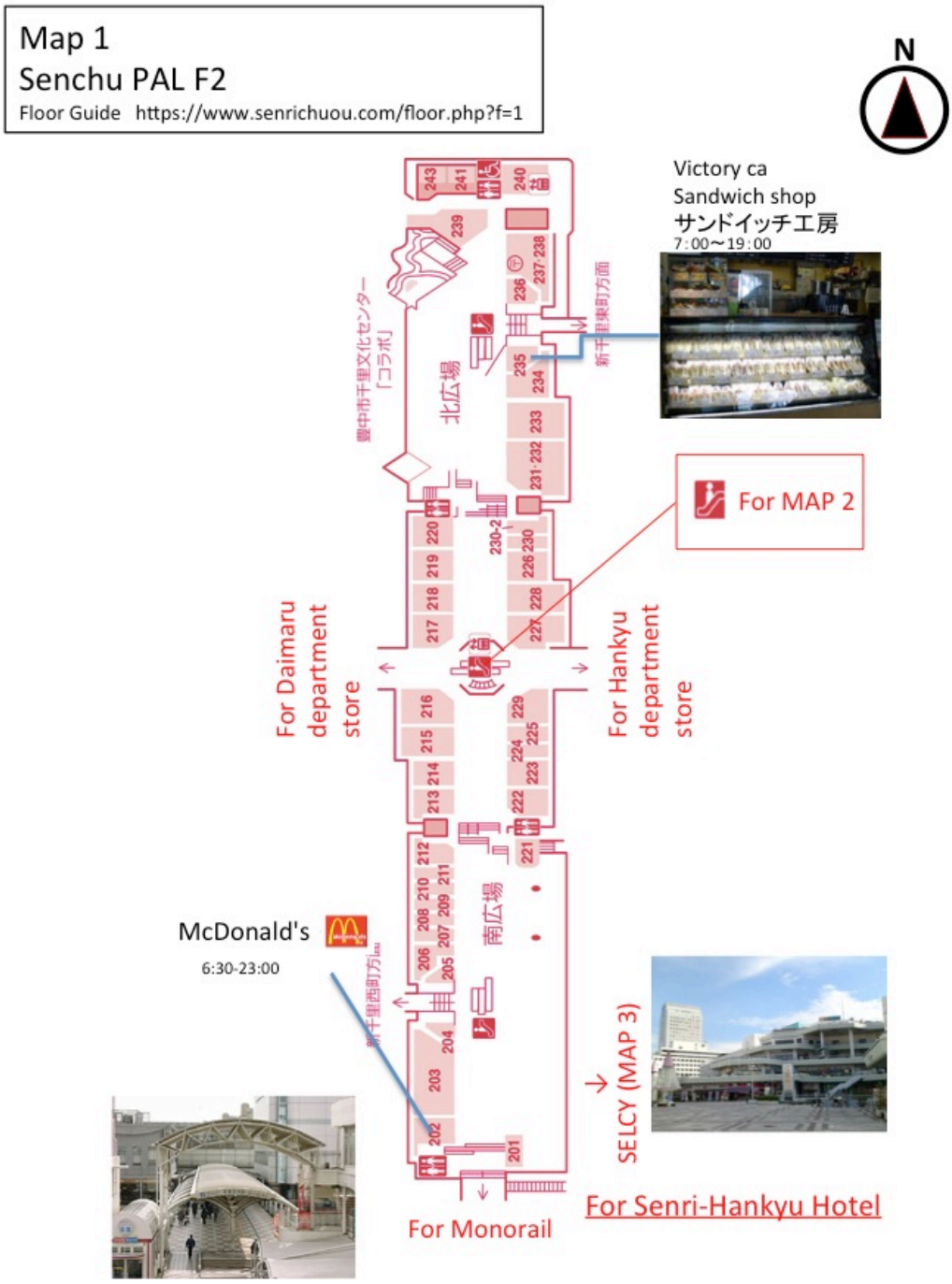
Registration:
The registration will be done at the workshop reception, which will be held on 18:00, Monday 20 (opening 17:30), March at Room Julin in Senri Hankyu Hotel. Registration fee is free.

Lunch and refreshments:
All the participants will get lunch boxes in lunchtime. Coffee, tea, and water will be served during breaks. There are restaurants and cafes in the shopping malls PAL and SELCY near Senri Hankyu Hotel (see the next page).

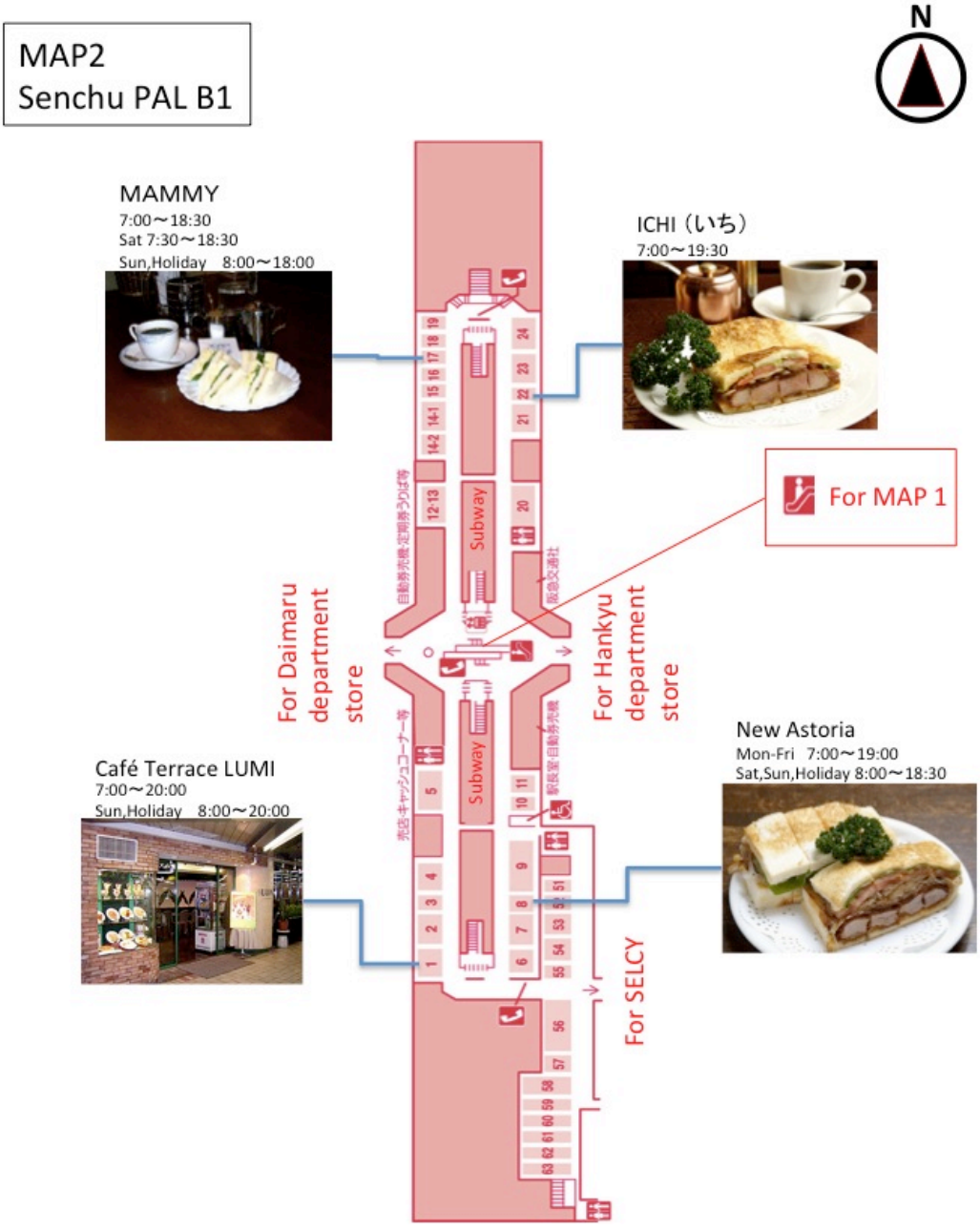
Official photo:
Official photo will be taken during the reception (18:00-20:00, Monday 20, March), which will be held on Monday 20 March.

Insurance:
The organizing committee is not responsible for illness or accidents that could occur during the workshop. We recommend you to check if your health insurance covers incidents happening while abroad.

Breakfast Cafe Maps:



MAP2
Senchu PAL B1



MAP 3
SELCY

MISTER DONUT
7:00～24:00

MOS BURGER
7:00～23:00

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SELCY

DOUTOR
Mon-Sat 7:15～21:00
Sun 8:00～21:00

Café Sanbankan
7:00～22:00

Program of Core-to-Core and Spintronics Workshop 2017

Start-Finish	No.	Speaker name (Affiliation, Country) *Title*

Monday, 20 March

Reception

1800-2000 (opening 1730) place: Room *Julin* at Senri Hankyu Hotel

Tuesday, 21 March

Opening

0850-0900		Hiroshi Katayama-Yoshida *Opening Address*

Session I: Introduction Chair: Hiroshi Katayama-Yoshida

0900-0920	01	Masaaki Tanaka (Univ of Tokyo, Japan) *Recent topics in semiconductor spintronics and ferromagnetic semiconductors*
0920-0940	02	Eisuke Abe (Keio Univ, Japan) *Quantum control and magnetic field sensing using nitrogen-vacancy centers in diamond*
0940-1000	03	Masafumi Shirai (Tohoku Univ, Japan) *Enhancement of voltage-controlled magnetic anisotropy by 5d transition-metal monolayer on ferromagnetic thin films*
1000-1015		Break

Session II: Methodology Chair: Hisazumi Akai

1015-1035	04	Danny Thonig (Uppsala Univ, Sweden) *First and higher order energy dissipation in atomistic magnetisation dynamics*
1035-1050	05	Tamio Oguchi (Osaka Univ, Japan) *Materials discovery for spintronics applications*
1050-1105	06	Ikutaro Hamada (NIMS, Japan) *Verification and validation of GW calculations for solids*
1105-1120	07	Takao Kotani (Tottori Univ, Japan) *Application of the QSGW method to power devices*
1120-1135		Break

Session III: Thermal properties Chair: Tatsuki Oda

1135-1150	08	Hiroshi Kohno (Nagoya Univ, Japan) *Microscopic approach to thermal spintronics theory*
1150-1205	09	Takashi Kimura (Kyushu Univ, Japan) *Efficient thermal spin injection based on metallic hybrid nanostructures*
1205-1220	10	Hiromi Yuasa (Kyushu Univ, Japan) *Enhancement of spin mixing conductance and spin Hall angle in spin Seebeck effect*
1220-1235	11	Yoshio Miura (Kyoto Ins Tech, Japan) *A first-principles study on voltage dependence of interfacial magnetic properties*
1235-1335		Lunch

Session IV: Spin control 1 Chair: Tetsuya Fukushima

1335-1355	12	Riccardo Mazzarello (Aachen Univ, Germany) *Ab initio simulations of phase-change materials*
1355-1410	13	Teruo Kanki (Osaka Univ, Japan) *Oxide Nano-Spintronics using Electronic Phase Transition*
1410-1425	14	Kensuke Kobayashi (Osaka Univ, Japan) *Symmetry control in the Kondo effect*
1425-1445	15	Alberta Bonanni (Johannes Kepler Univ, Austria) *Spin orbit coupling in nitride-based systems*
1445-1500		Break

Session V: Spin control 2 Chair: Yoshio Miura

1500-1515	16	Norikazu Mizuochi (Kyoto Univ, Japan) *Control of spin coherence of NV center in diamond*
1515-1530	17	Tatsuki Oda (Kanazawa Univ, Japan) *Magnetic interaction between the molecules attracting on week potential: approach along van der Waals density functional method*
1530-1545	18	Hisazumi Akai (Univ of Tokyo, Japan) *Non-equilibrium KKR Green's function method and its applications*

1545-1600	19	Teruo Ono (Kyoto Univ., Japan) *Dynamics of magnetic domain wall in ferrimagnets*
1600-1615		Break
Session VI: Transport		Chair: Susumu Yanagisawa
1615-1635	20	Shigeru Tsukamoto (Juelich, Germany) *Electron transport based on real-space finite-difference formalism for molecular spintronics*
1635-1650	21	Tomoya Ono (Univ of Tsukuba, Japan) *DFT study on carrier transport in devices*
1650-1705	22	Kohei Hamaya (Osaka Univ, Japan) *Spin transport in n-Ge and p-Ge*
1705-1720	23	Tatsuhiko Ohto (Osaka Univ, Japan) *Organic magnetoresistance (OMAR) studies by impedance spectroscopy*
1720-1735	24	Tsuyoshi Kimura (Osaka Univ, Japan) *Recent topic of electromagnetic effect*
1735-1750	25	Ryo Oshima (Kyoto Univ, Japan) *Spin transport via d-electrons at a $LaAlO_3/SrTiO_3$ interface*
Wednesday, 22 March		
Session VII: Catalysis		Chair: Ikutaro Hamada
0900-0920	26	Frank Abild-Pedersen (Stanford Univ., USA) *Efficient models for screening approaches in heterogeneous catalysis*
0920-0935	27	Naotaka Uchitomi (Nagaoka Univ. of Tech., Japan) *Room-temperature ferromagnetic behavior in $(Zn,Sn,Mn)As_2$ thin films based on magnetic percolation model*
0935-0950	28	Hidetoshi Kizaki (Osaka Univ, Japan) *First-principles investigation on the microscopic structures and their stability of Mn doped $ZnSnAs_2$*
0950-1005	29	Yuji Hamamoto (Osaka Univ, Japan) *Theoretical investigation on the catalytic activity of Pt clusters*
1005-1020		Break

Session VIII: Optical Chair: Hidetoshi Kizaki

1020-1040 30 Kee Joo Chang (KAIST, Korea)
Ab initio materials design by an inverse method based on conformational space annealing

1040-1055 31 Akira Oiwa (Osaka Univ, Japan)
Photon-spin Poincaré interface using a gate-defined quantum dots

1055-1110 32 Yasufumi Fujiwara (Osaka Univ, Japan)
Development of novel opto-spintronic functions in rare-earth doped semiconductors

1110-1125 33 Akira Masago (Osaka Univ, Japan)
Nanostructure in Eu-doped GaN

1125-1140 Break

Session IX: DMS Chair: Kazunori Sato

1140-1200 34 Lars Bergqvist (KTH Royal Ins Tech, Sweden)
Longitudinal spin fluctuations in atomistic simulations of magnetic alloys and compounds

1200-1215 35 Masayuki Toyoda (Tokyo Ins Tech, Japan)
Electronic Structure and magnetism of $Ba(TiO)Cu_4(PO_4)_4$

1215-1230 36 Shinji Kuroda (Univ of Tsukuba, Japan)
Synthesis and characterization of magnetic semiconductors based on II-VI and IV-VI compounds

1230-1245 37 Tetsuya Fukushima (Osaka Univ, Japan)
Materials Design of Magnetic Phase Change Materials by Order-N Screened KKR-Green Function Method

1245-1300 38 Hikari Shinya (Osaka Univ, Japan)
Magnetic mecahanism with nano-scale structure in Ge based DMS

1300-1400 Lunch

Session X: Thin film 1 Chair: Tamio Oguchi

1400-1420 39 Su-Huai Wei (Beijing Compt. Sci. Res. Center, China)
First-principle design of low dimensional materials for energy and spintronic applications

1420-1435 40 Hikaru Kawamura (Osaka Univ, Japan)

Frustration-induced spin textures

1435-1450	41	Tomoyasu Taniyama (Tokyo Ins Tech, Japan) *Control of magnetism in ordered FeRh*
1450-1510	42	Al-Jassim Mowafak (NREL, USA) *Multi-scale characterization of polycrystalline thin film PV devices*
1510-1525		Break

Session XI: Thin film 2 Chair: Takao Kotani

1525-1545	43	Biplab Sanyal (Uppsala Univ, Sweden) *Defects in 2D materials*
1545-1605	44	Myung Joon Han (KAIST, Korea) *Magnetism and spin-lattice-orbital interplay in nickelate, titanate, ruthenate heterostructures and thin films: First-principles perspective*
1605-1620	45	Kohji Nakamura (Mie Univ, Japan) *Materials design toward large perpendicular-magnetocrystalline-anisotropy thin films based on data-science*
1620-1635	46	Yoshishige Suzuki (Osaka Univ, Japan) *Voltage control of magnetic anisotropy, DMI and exchange interaction in ultrathin ferromagnetic films*

Closing

1635-1640

Abstracts

01

Recent topics in semiconductor spintronics and ferromagnetic semiconductors

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Ferromagnetic semiconductors (FMSs) have been intensively studied for decades as they have novel functionalities that cannot be achieved with conventional metallic materials, such as the ability to control magnetism by electrical gating or light irradiation [1-3]. Prototype FMSs such as (Ga,Mn)As, however, are always p-type, making it difficult to be used in real spin devices. Here, we demonstrate that by introducing Fe into InAs, it is possible to fabricate a new n-type electron-induced FMS with the ability to control ferromagnetism by both Fe and independent carrier doping. The studied $(In_{1-x},Fe_x)As$ layers were grown by low-temperature molecular beam epitaxy on semi-insulating GaAs substrates. Electron carriers in these layers are generated by independent chemical doping of donors. The ferromagnetism was investigated by magnetic circular dichroism (MCD), superconducting quantum interference device (SQUID), and anomalous Hall effect (AHE) measurements. With increasing the electron concentration (n = 1.8×10^{18} cm^{-3} to 2.7×10^{19} cm^{-3}) and Fe concentration (x = 5 - 8%), the MCD intensity shows strong enhancement at optical critical-point energies E_1 (2.61 eV), $E_1 + \Delta_1$ (2.88 eV), E_0' (4.39 eV) and E_2 (4.74 eV) of InAs, indicating that the band structure of (In,Fe)As is spin-split due to *sp-d* exchange interaction between the localized *d* states of Fe and the electron sea. SQUID and AHE measurements are also consistent with the MCD results. The Hall and Seebeck effects confirm the n-type conductivity of our (In,Fe)As samples. The electron effective mass is estimated to be as small as $0.03\text{-}0.175m_0$, depending on the electron concentration. These results reveal that the electrons are in the InAs conduction band rather than in the impurity band, allowing us to use the conventional mean-field Zener model of carrier-induced ferromagnetism [4]. This band picture is different from that of GaMnAs [5][6]. Our results open the way to implement novel spin-devices such as spin light-emitting diodes or spin field-effect transistors, as well as help understand the mechanism of carrier-mediated ferromagnetism in FMSs [7-14].

Furthermore, we demonstrate new phenomena in (In,Fe)As and its hetrerostructures: Novel crystalline anisotropic magnetoresistance with two fold and eight fold symmetry [7], and control of ferromagnetism by strain, quantum confinement, gate electric field and wavefunction engineering in quantum heterostructures with a (In,Fe)As quantum well [10-12]. Very recently, we have found a very intriguing phenomenon; sudden restoration of the band ordering associated with the ferromagnetic phase transition in the prototypical ferromagnetic semiconductor GaMnAs [15]. Also, we have successfully grown another narrow-gap p-type III-V-based FMS (Ga,Fe)Sb with high Curie temperature (T_C>300K) [16]. Combining different n-type and p-type FMSs will lead to new spin-related functionalities and devices.

This work was carried out in collaboration with Drs. S. Ohya, P. N. Hai, I. Muneta, L. D. Anh, M. Kobayashi, S. Sakamoto, and A. Fujimori. This work was partly

supported by Grants-in-Aid for Scientific Research, Project for Developing Innovation Systems of MEXT, and Spintronics Research Network of Japan (Spin-RNJ).

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02

Quantum control and magnetic field sensing using nitrogen-vacancy centers in diamond

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Electronic spins of nitrogen-vacancy (NV) centers in diamond possess long coherence times, and can be manipulated by microwave at around 2.87 GHz and be initialized and read out optically at ambient conditions. These excellent properties of the NV centers make them a leading candidate for ultra-sensitive, nanoscale magnetometers applicable to physical, biological, and medical sciences. It is also argued that the NV spins will be qubits for quantum information processing, once they are coupled coherently. The research on the NV centers is thus highly interdisciplinary, and various facets of science and technology must be considered and combined together.

In this talk, I will discuss our recent efforts to better control and utilize the NV spins, emphasizing our microwave engineering, spin physics, and materials science approaches. After briefly outlining the basics of the NV centers, I will introduce a circular microwave resonator we have developed recently [1]. It can create microwaves with arbitrary polarizations, and its resonance frequency is dynamically tunable between 2 and 3.2 GHz. Such polarization- and frequency-controlled microwaves enable the near-perfect selective excitation of the NV spins. I will then discuss the spin physics of high-density (10^{17} cm^{-3}) and narrow resonance-linewidth (200 kHz) NV ensemble we have created with a combination of CVD growth and helium ion implantation [2]. The study reveals an interaction between the NV spin and another electron spin, identified as a substitutional nitrogen donor spin, thereby demonstrates magnetic sensing on electron spins. The average distance between the NV spin and the donor spin is about 20 nm, suggesting that an NV spin positioned at 2 nm deep from the diamond surface can detect external nuclear spins placed on the surface. This has motivated us to develop a new technique to create “shallow” NV centers [3].

The work has been carried out with K. M. Itoh, K. Sasaki, J. Herrmann, K. Ito, H. Saito, J. Ishi-Hayase, and Y. Monnai of Keio University, H. Watanabe of AIST, T. Teraji of NIMS, and K.-M. Fu and E. Kleinsasser of University of Washington. The work at Keio University is supported by Spin-RNJ, JSPS KAKENHI (S) No. 26220602, JSPS Core-to-Core Program, and JST SENTAN Program.

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03

Enhancement of voltage-controlled magnetic anisotropy by 5d transition-metal monolayer on ferromagnetic thin films

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Voltage-controlled magnetic anisotropy (VCMA) is promising for reducing energy consumption in magnetization switching of magnetic tunnel junctions (MTJ). The magnetization switching by voltage pulse was demonstrated on Fe/MgO/FeCo and CoFeB/MgO/CoFeB MTJ [1, 2]. While the typical VCMA coefficients reported so far are 30-40 fJ/Vm [3, 4], larger values are required for the magnetization switching of MTJ with reduced dimensions. In this work, we theoretically investigated the VCMA of Fe(001) and Co(0001) films covered by the 5*d* transition-metal monolayer (ML) by means of first-principles density-functional calculations [5]. We evaluated the VCMA of TM(1ML)/bcc-Fe(4ML)/Cu(001)(5ML) and TM(1ML)/hcp-Co(4ML)/Cu(111)(5M L) films (TM = Hf, Ta, W, Os, Ir, Pt, Au). We found that the Ta/Fe, W/Fe, Os/Fe, Ir/Fe, Hf/Co, and Ir/Co films exhibit the VCMA larger than 100 fJ/Vm. In particular, the Ir/Fe film has the largest value, 263 fJ/Vm, which is about 8 times larger than that for the Fe surface. Among them, the Ir/Fe, Os/Fe, and Ir/Co films possess huge perpendicular magnetic anisotropy (PMA) greater than 10 mJ/m^2. We discuss the origin of the huge PMA and VCMA in the Ir/Fe film on the basis of the second-order perturbation of spin-orbit coupling [6]. We found that the PMA and VCMA are predominantly originated from the Ir layer. In particular, the spin-flip term between occupied majority-spin and unoccupied minority-spin states plays crucial role in the PMA of the Ir layer. On the other hand, both the spin-conservation term between occupied and unoccupied majority-spin sates and the spin-flip term between occupied minority- and unoccupied majority-spin states contribute to the VCMA.

This work was accomplished in collaboration with M. Tsujikawa and was funded by ImPACT Program of Council for Science, Technology and Innovation, Cabinet Office, Government of Japan.

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04

First and higher order energy dissipation in atomistic magnetisation dynamics

Danny Thonig, Olle Eriksson, and Manuel Pereiro
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An essential property of magnetic devices is the relaxation rate in magnetic switching which depends strongly on the damping in the magnetisation dynamics. Approaching the adiabatic limit, however, turned out to extend the Landau-Lifshitz-Gilbert equation by an inertia or higher order dissipation contribution [1]. Here, magnetic inertia is the resistance of the magnetic moment to relax, e.g., in ultra fast switching by an external magnetic field [2]. Both parameters are commonly taken as a phenomenological parameter, however large effort was spent recently to calculate Gilbert damping from first principles methods [3,4]. To the best of our knowledge, there were neither an ab initio nor experimental study that predict the size and relevance of magnetic inertia or higher order in energy dissipation.

We deduce the Gilbert damping and moment of inertia from the breathing band model [5] and apply it in the framework of a renormalised Green function tight-binding approach. Slater-Koster parameters were obtained by a genetic-algorithm and Monte Carlo optimisation with respect to first-principles results.

Our approach is applied to bulk Stoner magnets and is compared to recent experimental measurements [6]. It reveals that both the Gilbert damping and the moment of inertia are non-local, temperature- dependent tensorial quantities. Furthermore, our model predict even higher energy dissipation terms for both spin and lattice degrees of freedom. Moreover, atomistic magnetisation dynamics simulations reveal the importance of magnetic inertia in ultrafast relaxation processes.

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05

Materials discovery for spintronics application

Fumiaki Kuroda[1,2,3], Hitoshi Fujii[2,3], Tetsuya Fukushima[2,4,5,6], and Tamio Oguchi[2,3,4,5,6]
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Searching for novel materials with targeted electronic properties is crucial to success for the development of next-generation devices. Heusler alloys have attracted much attention for many years because they possess several interesting properties highly desired for spintronic, thermoelectric, and shape-memory device applications. Recently, spin-gapless semiconductors or semimetals (SGS) with Heusler structures have been proposed [1,2] and realized [3]. The electronic structure of Heusler based SGS is quite peculiar in the sense that semiconducting or semimetallic electronic nature takes place in one spin channel while the other spin bands are gapped, being possible alternative to the dilute magnetic semiconductors [4]. In this study, we searched for SGS materials in equiatomic quaternary Heusler alloys by using first-principles calculations with empirical band-filling rules [2] and succeeded to predict some alloys revealing SGS behavior. The electronic structure, structural stability, and magnetic properties of predicted Heusler based SGS as well as previously proposed and realized systems are discussed.

References

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06

Verification and Validation of GW calculations for solids

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Many body perturbation theory based on the GW approximation is a well established approach to compute quasiparticle energies of solids. Yet, systematic convergence tests as a function of basis sets, k-points and other numerical parameters entering the calculation are still lacking. We present a systematic convergence study of quasiparticle energies using a new release of the large-scale GW code WEST[1,2] including accurate k-point sampling of the Brillouin zone[3]. We also discuss comparisons with experiments.

References

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07

Application of the QSGW method to power devices

Y. Kamakura[1], R. Fujita[1], K. Konaga[1], Y. Ueoka[1], N. Mori[1], and T. Kotani[2]
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Wide bandgap semiconductors such as 4H-SiC and Diamond are greatly attractive for the application of next generation power devices. However, their device simulation models are still poor compared to those of Si. To overcome this situation, we are developing a Full-band Monte Carlo simulator (FBMC) where we obtain physical parameters by a first-principles method.[1]

Here we use a hybrid quasiparticle self-consistent GW (QSGW) method which is already proved to give accurate energy band structures for wide range materials.[2] In fact, we see that not only the experimental band gaps but also the experimental effective masses for 4H-SiC are described very well. The accurate band structure is key since it control acceleration of carriers under voltage applied.

Based on the band structure, we can calculate impact ionization rate (IIR) as the imaginary part of the self energy in the GW calculation [3]. The IIR is important quantity to determine the breakdown voltage of the power device via the Avalanche mechanism. The IIR together with the phonon scattering rates supplied to the FBMC, we can successfully calculate breakdown voltages consistent experiments.

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08

Microscopic approach to thermal spintronics theory

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Recently, thermal phenomena attract wide interest in the field of spintronics. In this presentation, I will talk about the microscopic calculation of spin torques induced by temperature gradients via conduction electrons [1, 2] as well as via magnons [3]. Special attention is paid to some theoretical issues on the treatment of temperature gradient and heat current.

These works have been done in collaboration with T. Yamaguchi, J. Fujimoto, Y. Hiraoka, M. Hatami, E. van der Bijl, R. Duine, and G. E. W. Bauer.

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09

Efficient thermal spin injection based on metallic hyvbrid nanostructures

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Generation, manipulation and detection of spin currents are important issues in the operation spintronic devices because a spin current plays an important role in spin-dependent transport and spin-transfer switching. Especially, pure spin current which is the spin current without accompanying the charge current is an attractive quantity for utilizing the spin current efficiently. Nonlocal spin valve measurements in laterally configured ferromagnetic metal (FM)/nonmagnetic metal (NM) hybrid nanostructures is a powerful means for evaluating the intriguing properties of pure spin current precisely. In this talk, I will introduce materials for the efficient generation and detection of the pure spin current and a structure for efficient control of the absorption property of the pure spin current.

In the first part, I will introduce the results on the efficient generation of pure spin current using CoFeAl. We show that CoFeAl alloy is an excellent material not only for the electrical spin injection but also thermal spin injection because of its favorable band structure as schematically shown in Fig. 1.[1] Moreover, the wireless microwave irradiation in the ferromagnetic metal is found to achieve the efficient thermal spin injection wirelessly.[2]

In the second part, I will introduce an unconventional lateral spin valve structure, in which the pure spin current flows in a FM/NM bilayer shown in Fig. 2. We show that the effective spin diffusion length can be modulated by the direction of the magnetization of the FM layer in the spin-current channel.

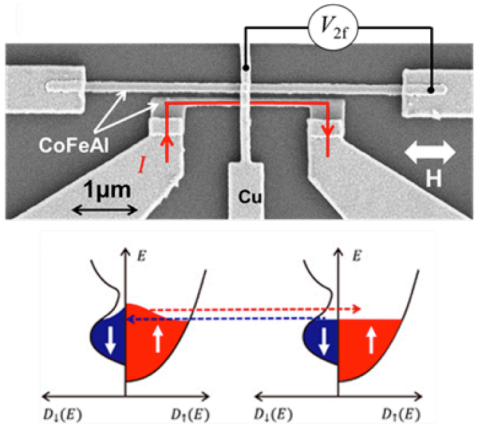

Fig. 1 Schematic illustration of the efficient spin injection together with a SEM image of lateral spin valve

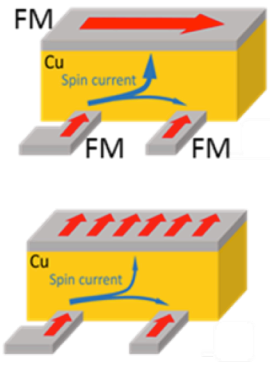

Fig. 2 Conceptual image of modulation of the spin absorption.

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Enhancement of spin mixing conductance and spin Hall angle in spin Seebeck effect

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The spin Seebeck effect and the inverse spin Hall effect generate the voltage by a temperature gradient in the ferrimagnetic oxide and nonmagnetic metal systems, which has a potential of thermoelectric generation by a uniform film [1-3]. However, the voltage is so small that we have to enhance it for application. We focus on two important physical parameters determining the voltage, that is , the spin Hall angle in the nonmagnetic metal and the spin mixing conductance at the interface between ferromagnetic oxide and nonmagnetic metal.

In order to increase the spin Hall angle, we applied the $Ta_{50}W_{50}$ alloy because it has the larger spin scattering than the simple b-Ta and b-W with the largest spin Hall anglein the reported materilas. Altohgh the YIG/$Ta_{50}W_{50}$ showed the slightly higher spin Seebeck voltage than YIG/Pt and YIG/W, it is lower than the voltage expected from the high spin scattering. Therefore, we took care of the spin mixing conductance and prepared YIG/Ru/$Ta_{50}W_{50}$ in order to restrain the oxidationa the interface with YIG. As a result, YIG/Ru/$Ta_{50}W_{50}$ showed the 2.4 times higher spin Seebeck voltage than YIG/Pt.

Next, we tried to increase it by inserteing the ferromagnetic metal layer at the interface YIG and Pt since it was theoretically reported that the spin mixing conductance depends on the magnetic density at the interface [4]. We inserted the several materials and YIG/FeCo/Pt showed the 1.5 times higher spin Seebeck voltage than YIG/Pt.

In conclusion, we increased the spin Seebeck voltage by two approaches; $Ta_{50}W_{50}$ with the large spin Hall angle and FeCo insertion with the high spin mixing conductance. It is one candidate to improve the spin Seebeck coefficient toward energy harvesting.

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A first-principles study on voltage dependence of interfacial magnetic properties

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Required properties for spintronic materials are the high spin polarization with low resistance, large perpendicular magnetic anisotropy with small magnetic damping constant α and a small saturation magnetization with large Curie temperature. In experiments, not only the magneto-crystalline anisotropy (MCA) but also the magnetic damping constant α of thin CoFeB layer in CoFeB/MgO/CoFeB MTJs can be modulated by the applied voltage[1]. Here, we report on the voltage dependence of magnetic damping constant and the MCA of thin Fe-layer using the first-principles calculations, and discuss the relation of the voltage effects between these two magnetic properties.

We calculated the magnetic damping constant and the MCA energy of free-standing thin Fe-layer and Fe/MgO(001) interfaces on the basis of the torque correlation model proposed by Kambersky[2]. We found that the magnetic damping constant α of free-standing thin Fe-layer increases with increasing the applied positive voltage (Increase of electron accumulation at surface), which is opposite voltage dependence as compared with the MCA energy of Fe-layer, corresponding to 7% of damping constant α can be changed by 1[V/nm]. The voltage dependence of magnetic damping of Fe-layer can be attributed to the spin-conservation term of torque operator. Large local density of states (LDOS) of surface Fe *d*(xy) and Fe *d*(yz,zx) orbitals around the Fermi level in the minority-spin state provide the large matrix elements of torque operator, providing the large magnetic damping constant of the spin conservation term. These LDOS increases with increasing the energy relative to the Fermi energy, leading to the large electric field dependence of the magnetic damping constant.

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12

Ab Initio Siulations of Phase-change Materials

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Phase-change materials (PCMs) can switch very rapidly and reversibly between the amorphous and crystalline phase at high temperature. Remarkably, the two phases are very stable at room temperature and exhibit pronounced optical and resistivity contrast. These unique properties have led to applications in data storage devices, such as rewritable optical devices (Blu-Ray Disc) and electronic non-volatile random access memories (PC-RAM). In these two classes of devices, heating is induced by laser irradiation and the Joule effect, respectively. The most important family of PCMs are the GeSbTe (GST) compounds which lie along the GeTe-Sb_2Te_3 pseudobinary line.

In this talk, I will present our recent work, based on density functional theory simulations, about the structural, electronic and kinetic properties of these materials. First, I will discuss the structural and electronic properties of the crystalline state of GST compounds. I will show that temperature-driven and stoichiometry-driven structural and metal-insulator transitions occur in these materials. Our large-scale simulations have elucidated the microscopic mechanisms responsible for these transitions. In particular, they have shown that the metal-insulator transitions are induced by vacancy disorder.

In the second part, I will focus on the structure, electronic structure and vibrational properties of quasi two-dimensional models and GST superlattices. These systems are relevant to interfacial PCMs, a novel family of PCMs which holds the promise of faster, energetically less demanding transitions. It turns out that that the switching mechanism of interfacial PCMs and the atomic structure of the two states is not understood, in spite of successful experimental demonstrations of memory devices based on these materials. If time permits, I will also discuss our recent efforts to understand the switching process by ab initio molecular dynamics simulations.

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Oxide Nano-Spintronics using Electronic Phase Transition

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Oxide materials with strongly correlated electrons show characteristic phenomena such as colossal magnetoresistance, metal-insulator transition and high-TC superconductivity, caused by strong coupling among spin, charge and orbital degrees of freedom. Among many correlated oxides, vanadium dioxide (VO_2) is the prototypical material, possessing a dramatic resistance and magnetism changes between a metallic state with paramagnetism and an insulating state with non-magnetism induced by dimerized singlet spins of vanadium atoms around 340 K. This metal-insulator transition (MIT) can be induced by a variety of external stimuli, such as thermal variation, lattice strain and electric field. Controlling of MIT by an electric field is especially expected toward the realization of Mott transistor. In this research, we fabricated VO_2 nano-wire channel-based field effect-transistors with a side-gate-type [1] and bilayer insulating gates [2].

VO_2 thin films were deposited on TiO_2 (001) substrate and Al_2O_3 (0001) substrate by using a pulsed laser deposition technique and formed VO2 nanowire patters with a variety of width through nanoimprint lithography method. The change rate in resistance (, defined as (Roff-Ron)/Roff, where Roff and Ron is the resistance of off-bias and on-bias states, respectively) on Al_2O_3 (0001) substrate is 0.4% at gate bias VG = 30 V, while the rate on TiO_2 (001) substrate is 4.5%, which is 10 times higher than that using Al_2O_3 (0001) substrate. It is considered that the huge difference was caused by obtaining single crystalline epitaxial VO_2 on TiO_2 (001) substrate. Furthermore, the change rate in resistance depend on wire width of VO_2 channels, that is, when reducing wire width of VO_2 channels from 3000 nm to 300 nm on TiO_2 (001) substrate, resistance modulation ratio enhanced from 0.7 % to 4.5 %. This indicated the advantage of nanowire and the modulation rate will be drastically enhanced in narrower width. In this workshop, we will show the detail data for difference of the change rate in resistance between in-plane polycrystalline VO_2 on Al_2O_3 (0001) substrate and of single crystalline VO_2 on TiO_2 (001) substrate, and width of VO_2 nanowire dependence of the change rate.

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Symmetry Control in the Kondo effect

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Kondo effect is a paradigm of strongly correlated many body state in condensed matter. It appears when conducting electrons interact with a localized one to screen any shared degenerate degree of freedom. Such a localized state can be realized in a carbon nanotube quantum dot where spin and orbital quantum number, which corresponds to clockwise or anti-clockwise wave functions, are degenerate. By tuning the degeneracies and filling factor, it is thus possible to investigate the usual twofold degenerate SU(2) Kondo effect as well as the four fold degenerate SU(4) state. Recently [1], we have investigated both symmetries near the unitary limit. Combining conductance and shot noise measurement, we have demonstrated that theory of Kondo effect can be safely extended out of equilibrium even in the SU(4) symmetry.

Here, using in-plane magnetic field up to 13 T to lift the degeneracy from four to two, we for the first time, provide a direct view of the crossover between SU(4) and SU(2) state for a constant filling factor of two electrons. A good agreement with theory is achieved for the evolution of the conductance and the Kondo temperature. Most importantly, we measured current fluctuations along this crossover, which show an increase of the non-equilibrium effective charge in perfect agreement with theory. This last result constitutes a direct evidence of the symmetry change and the enhancement of Kondo correlation with magnetic field [2].

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Spin-orbit coupling in nitride-based systems

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Nitride-based alloys, beside their importance for the lighting of the future and for the next generation of high power electronic devices, show remarkable features particularly attractive for spin-orbitronics, enabling, *e.g.*, spin-charge interconversion *via* spin-orbit coupling associated with inversion asymmetry and leading to a sizable Rashba field and piezoelectric properties.

We summarize how we have demonstrated the generation of pure spin current in bilayers Py/*n*-GaN:Si – at room temperature and through spin pumping [1]. We have found for *n*-GaN:Si a spin Hall angle $\theta_{SH}=3.03\times10^{-3}$, exceeding by one order of magnitude those reported for other semiconductors, pointing at III-nitrides as efficient spin current generators.

Moreover, we show – by direct magnetization measurements – the electrical control of the magnetization in (Ga,Mn)N [2]. In this dilute magnetic insulator the Fermi energy is pinned by Mn ions in the mid-gap region, and the Mn^{3+} ions show strong single-ion anisotropy. We have established that (Ga,Mn)N sustains an electric field up to at least 5 MV/cm, indicating that Mn doping turns GaN into a semi-insulating material. Under these conditions, the magnetoelectric coupling is driven by the inverse piezoelectric effect that stretches the elementary cell along the *c*-axis and, thus, affects the magnitude of the magnetic anisotropy. In this way, our work bridges two fields of research developed so far independently, namely: piezoelectricity of wurtzite semiconductors and electrical control of magnetization in hybrid and composite magnetic structures with piezoelectric components.

Finally, we provide an outlook on the perspectives for: (i) spin orbitronics in nitride Rashba semiconductors and nitride superconductors; (ii) electrical detection of spin Hall torque and Rashba torques in ferromagnetic/non-magnetic hybrid structures; (iii) for the role of proximity effects in ferromagnetic/non-magnetic hybrid structures.

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16

Control of spin coherence of NV center in diamond

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A single electron spin in a nitrogen-vacancy (NV) center in diamond has excellent properties such as single spin manipulation and readout at room temperature. Thus NV center has potentials to realize quantum information processing[1], nano-scale magnetic- and electric-fields sensors[2,3]. Coherence time of the NV-electron spin is very important because the performance of the applications is limited by the coherence time. A main decoherence source is fluctuating magnetic field induced by flipping of surround spins[4]. In this study, we focus on the electric-field effect on NV-electron spin because the impact of fluctuating magnetic field on NV-electron spin is suppressed by an external electric field and coherence time should be enhanced[3]. Here, we demonstrated an enhancement of the coherence time of the NV-electron spin by an external electric field.

Single NV centers were created in a CVD-grown diamond substrate by N^+ ion implantation. For applying electric field, electrodes were formed on the substrate. We observed electron spin resonance of single NV centers by optically detected magnetic resonance (ODMR) technique. A Ramsey (Hahn-echo) pulse sequence was employed in order to estimate the coherence time of T_2^{FID} (T_2^{echo}). The T_2^{FID} and T_2^{echo} were enhanced with increasing electric field. We analyzed the data based on spin Hamiltonian of NV-electron spin under magnetic- and electric-fields. The analysis indicated the measured T_2^{echo} under electric field was shorter than the expected value from the measured result at zero electric field. This may be caused by high-frequency electrical noise because such noise cannot be suppressed by the external electric field or be canceled out in the Hahn-echo sequence. This research was supported by CREST,JST and KAKENHI.

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17

Magnetic interaction between the molecules attracting on week potential: approach along van der Waals density functional method

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The magnetic interaction between constituent elements is important in magnetic materials on both the physical property and quantitative strength. The strength becomes critical, when it is comparable to those from the others, such as orbital hybridization interaction, spin-orbit interaction, van der Waals like interaction, etc. The practical construction for these potential energies is required for the studies which research and develop the spintronic devices with organic materials in the courses of theory or computational approach. As a starting point, the van der Waals density functional (vdW-DF) method [1] and the extensions to magnetic materials [2, 3] could be useful. Nowadays, such density functional approach can cover much large application systems, compared with the other accurate approaches, such as in the quantum chemistry. The former allows us to optimize the atomic or crystal structure easily in the development on the computational technique of N log N which is applied to the double integral of non-local interaction term.

The spin-dependent approaches of vdW-DF improves structural properties of the oxygen systems, such as molecular pair, solid oxygen, compared with the results of the conventional LDA/GGA approaches. Our calculation may also reveal the improvement on binding energy. These results convince us that the spin-dependent vdW-DF may be useful for the optimization on atomic structures in magnetic materials. As in the non-magnetic cases, the intermolecular potential at the distances around 2.5-4.0 angstrom becomes improved. I will discuss the results at these distances in the other magnetic application [4] in the talk.

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Non-equilibrium KKR Green's function method and its applications

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A scheme that combines the non-equilibrium Green's function method with the Korringa–Kohn–Rostoker (KKR) Green's function method is proposed [1]. The method is powerful since it is free from the well-know problem of Green's functions composed of a finite basis set. Also the various techniques that make use of the KKR Green's function method such as KKR-CPA can be directly implemented to the scheme. We report the some examples of the application of this method. First application is to Schottly contacts. Schottky contacts formed in metal-semiconductor junctions play an important role in semiconductor devices and integrated circuits. They have been intensively investigated for several decades not only for possible application to electronic devices but also for gaining a fundamental understanding of the Schottky barrier formation. Our results show that the Schottly barrier is formed between an undoped GaN and Al interface, showing that the asymmetric behavior of electron transport against the direction of bias voltage occurs in this system.

As the second example, we discuss the results of the application to magnetic junctions. The applicability of the method to systems where domain walls exist will be also discussed.

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19

Dynamics of magnetic domain wall in ferrimagnets

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Antiferromagnetic spintronics is an emerging research field which aims to utilize antiferromagnets as core elements in spintronic devices. Antiferromagnets are expected to show much faster spin dynamics than ferromagnets because they have higher resonance frequencies than ferromagnets. However, experimental investigations of antiferromagnetic spin dynamics have remained unexplored mainly because of the immunity of antiferromagnets to magnetic fields. Furthermore, this immunity makes field-driven antiferromagnetic DW motion impossible despite rich physics of field-driven DW dynamics as proven in ferromagnetic DW studies.

We show that fast field-driven antiferromagnetic spin dynamics is realized in ferrimagnets at the angular momentum compensation point TA. Using rare-earth–3d-transition metal ferrimagnetic compounds where net angular moment is nonzero at TA, the field-driven DW mobility remarkably enhances up to 20 km s−1T−1. The collective coordinate approach generalized for ferrimagnets and atomistic spin model simulations show that this remarkable enhancement is a consequence of antiferromagnetic spin dynamics at TA. Our finding allows us to investigate the physics of antiferromagnetic spin dynamics and highlights the importance of tuning of the angular momentum compensation point of ferrimagnets, which could be a key towards ferrimagnetic spintronics.

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Electron Transport Calculations based on Real-Space Finite-Difference Formalism for Molecular Spintronics

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The computing unit cells used for electron transport calculations are generally composed of not only scattering objects but also parts of electrodes, and hence, the computation is more expensive than that for the electronic structures of bulk systems. In particular, the transport calculations for molecular junctions require larger computing unit cells in comparison to those for bulk interfaces. For such large-scale systems, the real-space finite-difference (RSFD) formalism and pseudopotential methods are well known to be suitable in terms of computational efficiency on massively parallel computers. So far, we have developed a ballistic electron transport calculation method, called juTrans, based on the RSFD formalism and the projector-augmented wave (PAW) pseudopotentials. As compared to other electron transport calculation methods using localized-orbital basis sets, our method is completely free from choosing basis functions. On the other hands, it is still expensive because of the large degree of freedom in solving the Kohn-Sham equation for scattering wave functions.

Our approach to the problem on the computational cost is to reduce the degree of freedom to the requisite minimum without any approximation and losing accuracy. We have found that a block of the Hamiltonian matrix is rank-deficient due to the separable form of the PAW pseudopotentials, and can be transformed into a size-reduced and regular matrix by using the singular value decomposition. As the consequence of the matrix transformation, the overbridging boundary matching formula for scattering wave functions is expressed as smaller linear equations. The reduction of the matrix size turned out to be more than 60%, and the memory consumption for storing the coefficient matrices is reduced by more than 80%.

In the presentation, we are going to show not only the development of the method but also some transport calculation results for molecular spintronics. We examine the electron transport properties of sandwich compounds containing magnetic elements. More specifically, each of ferrocene, cobaltocene, and nickelocene is placed between a couple of non spin-polarized electrodes, and the spin-dependent electron transmission spectra are investigated.

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DFT study on carrier transport in devices

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DFT attracs attention as one of the most important practical tools to investigate or determine the electronic, structural and many other properties of nanostructures in physics, chemistry, and materials science. A typical trend observed is that we need to deal with increasingly more complex systems characterized by many atoms of different chemical nature in open structures and of low symmetry. This path is supported by the increasing availability of powerful computers. The developments of computers show that we have to cope with massively parallel computer architectures dealing with thousands of cores. Therefore, it is important to develop calculation methods whose applicability scales with the available processes.

The real-space finite-difference (RSFD) method[1,2] of first-principles calculations, where all computations are performed in real space, is a method that has the potential to scale with massively parallel computers and has this potential without compromise on the accuracy and thus should be superior to conventional plane wave methods. Further advantages of RSFD method are that (i) the computational costs involved in calculating the projectors of pseudopotentials can be reduced when the calculations are carried out in real space. (ii) The grid spacing should be narrowed in order to improve the computational accuracy. A procedure is simple and definite. (iii) Boundary conditions are not constrained to be periodic, e.g., combinations of periodic and nonperiodic boundary conditions for surfaces and wires are included straight forwardly. In particular, point (iii) is significantly advantageous for electron-transport calculations because semi-infinite boundary condition, in which a crystalline bulk is infinitely repeated toward inside of the electrode and is faced the transition region at the opposite side, is indispensable for the direction in which electrons flow.

We have developed a first-principles calculation code, RSPACE,[2] based on the RSFD method. In this talk, I present a couple of studies for electronic-structures and transport properties of nano-devices[3] using RSPACE.

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Spin transport in *n*-Ge and *p*-Ge

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Because of the future intrinsic limits of the shrinking of silicon (Si)-based conventional complementary metal-oxide-semiconductor (CMOS) transistors, one should develop novel devices with additional functionalities other than the miniaturization of the channel length. Since one of the most important technologies is an enhancement in the current drivability, germanium (Ge) having the higher carrier mobility than Si is expected to be a new channel material in next-generation CMOS transistors.1,2) To further enhance the functionality of the Ge electronics devices, we have also focused on the spin-based electronics (spintronics), which enables us to significantly improve device performances because of its nonvolatility, reconstructibility, low power consumption, and so forth.3) Here we present our recent work on electrical spin injection and detection in *n*-Ge and *p*-Ge by using high-quality Heusler-alloy electrodes to integrate spintronic technologies into Ge electronics.

Using molecular beam epitaxy (MBE) techniques, we have established highly ordered Heusler alloys on Ge(111) and we have obtained high-quality Heusler-alloy/Ge heterointerfaces.4) To achieve electrical spin injection and detection without using insulator tunnel barriers, we used Schottky tunnel barriers. 5) For *n*-Ge, lateral spin-valve (LSV) devices with Heusler-alloy electrodes were fabricated. From nonlocal voltage measurements,6) we evidently detected spin signals and Hanle-effect curves for *n*-Ge at low temperatures,7) and recently observed the spin signals up to room temperature in Co2FeAl0.5Si0.5/*n*-Ge LSVs.8) Also, we clarified the spin relaxation mechanism in *n*-Ge.7,8) For p-Ge, we demonstrated nonlocal spin transport through the *p*-Ge (~40 nm) layer by using an LSV structure with a Cu channel.9) Very recently, in vertically stacked CoFe/*p*-Ge (20 nm)/Fe3Si trilayer structures, we observed two-terminal magnetoresistance curves meaning spin-dependent transport through the *p*-Ge layer.10) Temperature- and bias-voltage dependence of the spin-dependent transport in the *p*-Ge layer will be presented.

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Organic magnetoresistance (OMAR) studied by impedance spectroscopy

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Organic magnetoresistance (OMAR) has been observed for various organic semiconductors sandwiched between non-magnetic electrodes at room temperature and at low magnetic field (typically a few tens mT). These simple observation conditions make OMAR a promising candidate for applications such as the fabrication of magnetometers. The OMAR effect is explained by several models: a “single-carrier” model based on biporalon and “double-carrier” models based on electron-hole pairs or excitons. In most devices, several types of OMAR coexist, which makes it difficult to identify the underlying mechanism. We used impedance spectroscopy to elucidate the OMAR mechanism in our devices. In the case of the poly(3-hexylthiophene-2,5-diyl) (P3HT) diode, the capacitance deduced from the impedance data indicate that the OMAR was explained by the single-carrier (bipolaron) model at lower bias voltages and double- carrier models at higher bias voltages[1]. Furthermore, the effect of traps caused by the roughness at the interface between the hole injection layer [poly(3,4-ethylenedioxythiophene): poly(styrenesulfonate): PEDOT:PSS] and the phenyl-C61-butyric acid methyl ester (PCBM) on OMAR has been revealed from the results of impedance spectroscopy[2]. We demonstrated that the interface is important for controlling OMAR, and that the combination of OMAR measurement and impedance spectroscopy is helpful for clarifying the processes in the devices.

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Multiple order parameters and their domain control in magnetoelectric multiferroics

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

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

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Spin transport via *d*-electrons at a $LaAlO_3/SrTiO_3$ interface

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A two-dimensional electron gas (2DEG) at $LaAlO_3/SrTiO_3$ (LAO/STO) interfaces consists of *d*-orbital electrons [1]. A *d*-electron is localized and a source of magnetism in 3*d* transition metals, however, this special *d*-2DEG enables us to investigate a *d*-electron as a carrier for charge and spin. An experimental demonstration of spin transport via *d*-electrons is a challenge for a new approach to the spin transport with an electron and conventional understanding for their *d*-electrons character such as their short-range spin coherence. Here, we demonstrate the spin transport in *d*-2DEG at LAO/STO interfaces at room temperature.

We fabricated $Ni_{80}Fe_{20}$ (Py) and Pt wires, separated by 1 mm, on LAO/STO substrate. Spins are injected from the Py wire into LAO/STO interfaces under the ferromagnetic resonance condition (spin pumping [2,3]) and absorbed in the Pt wire through LAO/STO interfaces. Then, absorbed spins are observed as the electromotive force on inverse spin Hall effect (ISHE) [4]. Figure 1(a) shows the electromotive force from the Pt under the resonant field (m_0H_{FMR}). The sign of the electromotive force was reversed by reversing the direction of spin polarization (applied magnetic field direction q_H = 0° and q_H = 180°) and by replacing detector material from Pt to Ta which possess a negative spin Hall angle q_{SHE} (Figure 1(b)). This long-range spin transport at *d*-2DEG can be confirmed by two model calculations, the signal dependence on the transport length and the Gilbert damping measurement.

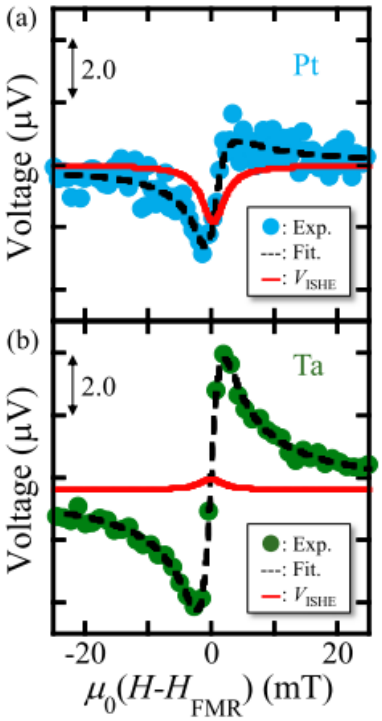

Fig. 1 The electromotive forces from (a) Pt and (b) Ta electrodes under the resonance field.

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Efficient Models for Screening Approaches in Heterogeneous Catalysis

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Sustainable energy solutions for the future will have to rely heavily on the energy influx from the sun. The need to have access to energy when and where we need it requires storing that energy in an appropriate form. The transformation of solar energy into chemicals like fuels that can be transported within an existing infrastructure is one convenient way of storing it. The efficiency of such transformation will require catalysts that are optimized for specific reactions, and we will need to find new and more efficient catalysts for a number of processes, if we are to successfully synthesize fuels from sunlight.

Energy correlations in heterogeneous catalysis provide and efficient way of screening a large number of catalysts for their activity and selectivity as they provide thermodynamic as well as kinetic information based on a simple set of descriptors.[1,2] The kinetic data still involves significant computational efforts and by specifically looking at ways to extend the relations to adsorbates far from their equilibrium structure we have derived models that can relate the variations in the scaling parameters to the variation in the adsorbate-surface bond strength as the structure of the adsorbate changes. The method provides a simple way of obtaining activation barriers based on very few calculations and it explicitly incorporates the variations in the transition state structure across different surfaces.[3,4]

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Room-temperature ferromagnetic behavior in (Zn,Sn,Mn)As2 thin films based on magnetic percolation model

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$ZnSnAs_2$ is a pnictide II-IV-V_2 chalcopyrite semiconductor in the bulk form with a band gap of 0.73 eV at 300 K. It is a tetrahedrally bonded ternary compound with a c/a lattice parameter ratio of 2.0, and crystallizes into either an ordered chalcopyrite or a disordered sphalerite (zinc-blende type) structure. The special advantage of this compound is having a lattice constant almost matched to that of InP. In recent years, $(Zn,Sn,Mn)As_2$ thin films have attracted interest because of their ferromagnetic behavior above room temperature and their promise of compatibility with InP-based heterostructures [1, 2].

In this work, the relationship between several Mn doping concentrations of up to 24 cation percent (cat.%) and Curie temperature (TC) is studied for $(Zn,Sn,Mn)As_2$ ferromagnetic semiconductors which were epitaxially grown on InP substrates by molecular beam epitaxy (MBE). It is found that ferromagnetic properties with Curie temperature of 334 K appear abruptly when Mn doping concentration increases to about 4 cat.% Mn. Mn distributions in $(Zn,Sn,Mn)As_2$ thin films are then investigated using three-dimensional atom probe tomography (APT), in which isoconcentration surfaces of Mn in the range of 0.5–3.0 atomic percent (at.%) are analyzed. As the Mn concentration in the $(Zn,Sn,Mn)As_2$ thin films is increased, Mn-As clusters with random size and position outspread, leading to a macroscopic ferromagnetic transition across the entire sample. Based on magnetic percolation model, the value of 2 at.% Mn concentration is interpreted as the magnetic percolation threshold for ferromagnetism in $(Zn,Sn,Mn)As_2$. Ferromagnetic properties as a function of annealing temperature can also be understood on the basis of magnetic percolation model by referring to theoretical works reported by several groups. We propose that the behavior of ferromagnetism in $(Zn,Sn,Mn)As_2$ can be well-explained within the framework of magnetic percolation model.

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Firs-Principles Investigation on the microscopic structure and their stability of Mn-doped $ZnSnAs_2$

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For realizing semiconductor spintronics, researchers have tried to synthesize dilute magnetic semiconductors (DMS) with high Curie temperature (T_C). So far, III–V based DMS such as GaMnAs have been investigated from both experimental and theoretical points of view as promising spintronics materials[1-3].

Recently, there have been renewed efforts and initiatives directed towards the study of Mn-doped II–IV–V_2 with the reported above-room-temperature ferromagnetism in $ZnSnAs_2$:Mn[4-6]. Moreover, it has been reported that $ZnSnAs_2$; Mn has a sphalerite structure in which Zn- and Sn-site represent disordered systems[7].

In this work, in order to elucidate the magnetic properties, we have investigated electronic structure and estimated the T_C in Zn(Sn,TM)As_2 and (Zn,TM)$SnAs_2$, TM = V, Cr, Mn, Fe, Co, Ni, using *Ab-initio* calculations within local density approximation (LDA).

As a result, we can expect to obtain the half-metallic, high-spin ferromagnetic state and high-T_C in Zn(Sn, V)As_2, Zn(Sn, Cr)As_2, Zn(Sn, Mn)As_2, (Zn, V)$SnAs_2$ and (Zn, Cr)$SnAs_2$ as shown in Figs. 1 and 2. In view of experimental results of room temperature ferromagnetism in Mn-doped $ZnSnAs_2$, it is in good agreement with that if we can control a selective Mn-doping at Sn-sites. Finally, we would like to discuss the stability of Mn-doped $ZnSnAs_2$ system on the microscopic structure.

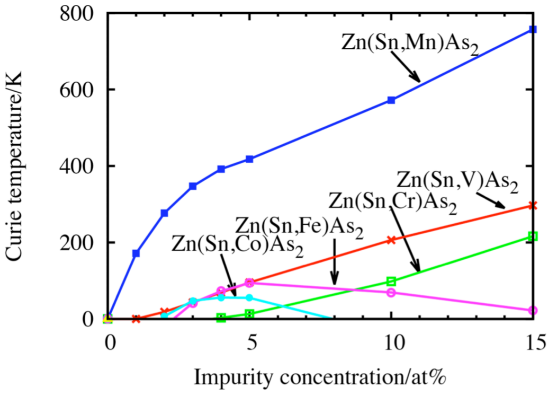

Fig. 1 Estimated *T*c in Zn(Sn,TM)As_2 within LDA.

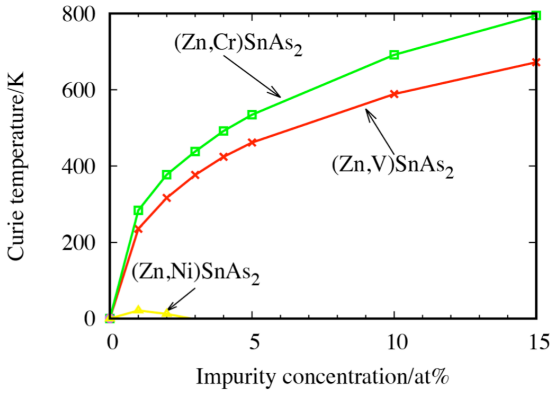

Fig. 2 Estimated *T*c in (Zn,TM)$SnAs_2$ within LDA.

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Theoretical investigation on the catalytic activity of Pt clusters

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Graphene, atomically thin two-dimensional material composed of a honeycomb lattice of carbon atoms, has drawn keen attention since its experimental realization, due to the peculiar electronic and structural properties. Nowadays, the applications of graphene to various industries have been explored extensively, among which one of the most promising candidates is the usage of graphene as a support material of metallic cluster catalysts. Experiments have demonstrated that Pt clusters deposited on graphene exhibit higher catalytic activity than on other carbon substrates such as carbon black and carbon nanotubes [1]. Similar phenomena can be found for Pt clusters supported on highly oriented pyrolytic graphite (HOPG), in which reduction of CO desorption temperature from the Pt clusters has been observed with temperature programmed desorption measurements [2,3]. The analogy between the HOPG surface and graphene suggests that CO poisoning tolerance plays an essential role also for Pt clusters on graphene. Despite these experimental evidences, however, little has been understood about the microscopic mechanism of the enhanced catalytic activity of Pt clusters on graphene. To gain theoretical understanding of these phenomena, we here investigate CO adsorption on Pt clusters on defective graphene as shown in the figure below. We show that, unlike Pt clusters on pristine graphene, those deposited on graphene vacancies induce large electron transfer form Pt clusters to graphene, which is accompanied by a significant change in the electronic states of the Pt clusters. As a result, CO adsorption energies on these Pt clusters become much smaller than those on isolated Pt clusters and Pt surfaces, which can be a possible scenario for the enhanced catalytic activity observed experimentally.

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Ab initio materials design by an inverse method based on conformational space annealing

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Based on quantum theory, understanding and predicting the properties of materials composed of atoms are very challenging in materials science. Recently, the so-called inverse method of materials design has drawn much attention, where specific material properties are initially assigned and target materials are subsequently found. Recently, we have developed a protocol for computational materials design, called AMADEUS (*Ab initio* MAterials DEsign Using cSa), in which the conformational space annealing (CSA) algorithm for global optimization is combined with first-principles density functional calculations [1]. Here we discuss the implementation and efficiency of our new scheme for materials design and show the results of applications for searching for Si and C allotropes with direct band gaps [2-4], B high-pressure phases [5], and novel materials with exotic electronic properties [6].

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Photon-spin Poincaré interface using a gate-defined quantum dot

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Since the electrically defined GaAs quantum dots (QDs) have already proven their suitability for solid state qubits [1], quantum state conversion from single photons to single electron spins in the gate-defined QDs and the entanglement among electron spins in distant QDs are indispensable technologies for long distance quantum communications [2]. Toward this goal, the angular momentum conversion from circularly polarized single photons to single electron spins in a double GaAs QD has been realized [3]. For an entanglement distribution and practical applications, further developments are needed. Here, we discuss the routes to enhance the conversion efficiency from photons to electrons and the transport through a SiGe self-assembled QD.

First, from the FDTD simulations, we show that the surface plasmonic antenna combined with a gate-defined QD formed in an AlGaAs/GaAs quantum well increases the transmission of light though a center aperture [4]. Based on the simulation, the devices were fabricated. Second, time-resolved Kerr rotation in a (110) GaAs quantum well, in which heavy hole states show Zeeman splitting under in-plane magnetic field [5], has been measured to verify the quantum state conversion using heavy hole states.

Recently, Si-based QDs are extensively studied as a promising candidate of spin qubits because of their long spin coherence time [6]. We have investigated the transport properties though a SiGe self-assembled QD toward a quantum memory for quantum repeaters and have observed Kondo effect.

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Development of novel opto-spintronic functions in rare-earth doped semiconductors

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We have intensively investigated rare-earth (RE)-doped III-V semiconductors grown by atomically controlled organometallic vapor phase epitaxy (OMVPE) and fabricated new types of functional devices using the materials. We have already succeeded in growing Eu-doped GaN layers with high crystalline quality, and have demonstrated for the first time a low-voltage current-injected red emission due to the intra-*4f* shell transitions of Eu^{3+} ions from p-type GaN /Eu-doped GaN/n-type GaN light-emitting diodes (LEDs) with an applied voltage of as low as 3 V [1]. The Eu^{2+} state is very attractive for future application of Eu-doped GaN because it has a potential to emit blue/green light due to the 5*d*-4*f* transition and to provide a magnetic moment. The valence state of Eu ions can be controlled by adjusting conditions of OMVPE growth and impurity codoping. In GaN grown at lower temperatures, the Eu^{2+} state was obviously revealed by XANES and its volume ratio to the Eu^{3+} exhibited a maximum at 700ºC. The volume ratio could also be controlled by the codoping of Si and/or O, and it increased linearly with electron concentration. The samples exhibited super-paramagnetism due to quite small clusters consisting of three Eu^{2+} ions at low temperature. Furthermore, magnetoresistance measurements indicated the presence of the *s-f* exchange interaction between conduction electrons and Eu^{2+} ions. These results suggest strongly a possibility for Eu-doped GaN to create novel devices for combined applications of optoelectronics and spintronics.

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Nanostructure of Eu-doped GaN

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We investigate nanostructural dependence of magnetic and optical properties of Eu-doped GaN using multi-scale modeling combining an ab initio calculation and two kinds of Monte Carlo simulations. [1-4] This is because Eu-doped GaN is known as a luminescent material emitting red light, ferromagnetic or superparamagnetic behavior has been observed in Eu-doped GaN, and self-organized nanostructures have been observed in a similar system: Er-doped GaSb. [5-7] Nevertheless, little has been reported for the relations between the nanostructures, the magnetic, and optical properties in rare earth doped semiconductors.

In this study, we simulate nanostructures when Eu atoms are doped into a cubic GaN crystal. This simulation provides us with various nanostructures depending on annealing time, temperature, and methods. These nanostructures are quantum dots called Dairiseki-phase and nano rods called Konbu-phase. [7] These systems show paramagnetic and superparamagnetic behaviors when the external magnetic field is applied in our simulations.

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Longitudinal spin fluctuations in atomistic simulations of magnetic alloys and compounds

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We have constructed a general framework for atomistic simulations of multi-component random alloys and compounds including longitudinal fluctuations. The main ingredients consist of mapping total energies from electronic structure calculations for a number of fixed magnetic moments in both the low temperature ferromagnetic limit and the high temperature paramagnetic limit. The model is then "exact" in the both limits and interpolating between the two at intermediate temperatures. Within the model, each magnetic moment magnitude is allowed to change that approximately corresponds to Stoner excitations in real materials and the model is constructed in such a way that the strength of the exchange energy is independent on the starting reference state of the mapping, which is typically not the case in normal cases.

The computational framework has been implemented in Monte Carlo and applied to the elemental transition metals Fe, Co and Ni, together with the binary random alloys Py and Fe_{1-x}-Co_x. Regarding the Curie temperatures, with the exception of Fe, the calculated values are in general slightly underestimated compared to experiments. However, the values are found rather insensitive from the starting reference state which is an attractive feature lacking in "normal" simulations for most materials. The simulations do qualitatively describe rather well the high temperature magnetic properties such as the correlation where excellent results compared to experiments are found.

By introducing a more advanced treatment of changing the phase space measure that includes a Jacobian factor within the Monte Carlo, significant improvements to the thermodynamics are found and even notoriously difficult systems such as Ni and Ni-based alloys are described rather well, as well as alloys having induced moments such as $Fe_{1-x}Pd_x$.

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Electronic Structure and magnetism of $Ba(TiO)Cu_4(PO_4)_4$

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Noncollinear magnetic orders such as multipole or toroidal moments have been theoretically proposed as drivers for magneto-electric (ME) effects such as magnetic-field-induced polarization or electric-field-induced magnetism. This mechanism has been experimentally confirmed in several materials with magnetic toroidal moments, however not with magnetic multipole moments. Recently, Kimura and co-workers have succeeded to observe ME activity in a newly synthesized material, $Ba(TiO)Cu_4(PO_4)_4$ [1,2]. From their experimental observation and theoretical analysis, they concluded that the ME activity is induced by its magnetic quadrupole moments. However, the underlying mechanism how the quadrupole moments are realized has not been fully understood. Furthermore, unfortunately, macroscopic ME effect is not observed because of the antiferroic stacking of the magnetic quadrupole moments. Therefore, in search for the first-ever material that exhibit macroscopic ME effect induced by magnetic multipole moments, it is important to study the detailed properties of $Ba(TiO)Cu_4(PO_4)_4$ so that it will be possible to find a way to switch the antiferroic stacking of the moments to ferroic. In this study, the electronic and magnetic properties of $Ba(TiO)Cu_4(PO_4)_4$ have been investigated by using first-principles density functional theory (DFT) calculations and classical Monte Carlo simulations. The magnetic exchange coupling constants were calculated from the total energy variation between different magnetic spin configurations. Spin canting effect was also estimated by calculation with spin-orbit coupling. Our results reasonably reproduce the experimentally observed magnetic properties such as the transition temperature and the magnetization (*M*-*H*) curve. We will discuss about what is the dominant magnetic interactions in $Ba(TiO)Cu_4(PO_4)_4$ and how they are modified when replacing ions and applying external pressure.

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Synthesis and characterization of magnetic semiconductors based on II-VI and IV-VI compounds

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Realization of ferromagnetism in semiconductors has been regarded as indispensable for application of spintronics. Many efforts have been devoted to search novel materials of diluted magnetic semiconductors (DMSs) exhibiting ferromagnetism. Up to now, DMSs consisting of various combinations of host semiconductors and magnetic elements have actually been synthesized and some them has been claimed to exhibit ferromagnetism at room temperature. After extensive studies on various DMS materials, it has been recognized that the magnetic properties of synthesized crystals depend on how the magnetic impurities are incorporated in the host crystal[1]; the magnetic impurities are distributed randomly on the substitutional site of the host crystal or they aggregate either in the form of the same crystal structure of the host matrix or as precipitates of an extrinsic phase of different crystal structure[2]. In this presentation, we will introduce our recent studies on DMSs based on II-VI and IV-VI compounds, (Zn,Fe)Te and (Sn,Mn)Te. We have made atomic-scale structural analyses on thin films grown by MBE and have investigated how the incorporation of the magnetic impurities are correlated with the magnetic properties.

(Zn,Fe)Te thin films were grown on a GaAs substrate by MBE equipped with elemental sources of Zn, Te, Fe. Among various MBE growth conditions, the ratio between the amount of supply of Zn and Te fluxes was found to dominate the structural and magnetic properties[2,3]; the films grown with an excess supply of Zn flux (Zn-rich growth) exhibit superparamagnetic behaviors with a high apparent Curie temperature[3], while the films grown in the excess of Te flux (Te-rich growth) exhibit paramagnetic behaviors[2]. Structural analysis using TEM revealed the Fe-aggregated regions of nano-scale columnar shape are formed along the growth direction in the films grown in the Zn-rich condition. The XAFS measurement at the Fe K-edge suggests that the Fe-aggregated regions are composed of a Zn-Fe compound, to which the observed superparamagnetic behaviors could be attributed.

(Sn,Mn)Te arouses our interest not only in the realization of ferromagnetism but also from the viewpoint of the effect of magnetic impurities on the surface state in topological crystalline insulator SnTe[5]. (Sn,Mn)Te thin films were grown on BaF_2 or CdTe by MBE using SnTe and Mn sources. The hole density in the films was controlled by supplying Te flux in addition to SnTe flux. The films grown without additional supply of Te flux, having relatively low hole densities of the order of $10^{20}cm^{-3}$, exhibit paramagnetic behaviors with antiferromagnetic interaction between Mn. However, a ferromagnetic feature starts to appear with the increase of the hole density up to $10^{21}cm^{-3}$. This result suggests the onset of ferromagnetic interaction between Mn due to the hole-mediated mechanism.

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Materials Design of Magnetic Phase Change Materials by Order-N Screened KKR-Green's Function Method

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The purpose of this work is to investigate the electronic structure and magnetic properties of the transition metal (TM)-doped Ge-Sb-Te (GST) systems by the all-electron full-potential screened Korringa-Kohn-Rostoker Green's function method [1]. In particular, we clarify the stable magnetic state of each TM doped GST by calculating the magnetic exchange interactions between the TM impurities. We employ a quite large supercell with 1000 atoms to avoid the artificial Coulomb interaction by the periodicity: the stoichiometry is $Ge_{200-x}Sb_{200-y}TM_{x+y}V^{c}_{100}Te_{500}$ and x+y is the number of TM impurities. Of course, a lot of computational costs are required to calculate such large system including the complex magnetic structure. Therefore, the KKRnano program package developed by Zeller and Thiess, which is optimized by a massively parallel linear scaling (order-*N*) all electron algorithm, is applied to our model of the magnetic GST. It is found that ferromagnetic states are favorable in the cases of V and Cr doping, due to the double exchange mechanism, whereas antiferromagnetic superexchange interactions appear to be dominant for Fe- and Mn-doped GST. The ferromagnetic interaction is particularly strong in the case of Cr. As a result, high Curie temperatures close to room temperatures are obtained for large Cr concentrations of 15 %.

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Magnetic mechanism with nano-scale structure in Ge based DMS

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For the discovery of carrier induced ferromagnetism in dilute magnetic semiconductors (DMS), many efforts have been devoted to the characterization and understanding of these materials, with the aim of realizing semiconductor spintronics [1,2]. Among them, Ge-based DMSs have recently attracted a lot of interests. There are many advantages in these DMSs from practical applications and consistencies with the general semiconductor technology point of view, compared to the typical III-V and II-VI type magnetic semiconductors, such as (Ga,Mn)N, (Ga,Mn)As, (Zn,Cr)Te, etc. Devillers *et al*. indicated that in $Ge_{1-x}Mn_x$, the Mn-rich nano-structure generated by the spinodal nano-decomposition plays an important role for the ferromagnetic Curie temperature (T_C) [3]. Moreover, the structural property of the nano-structure strongly depends on the crystal growth temperature. Wakabayashi *et al*. succeeded in the enhancement of T_C in $Ge_{1-x}Fe_x$ up to 210 K by controlling the annealing temperature, and showed that the inhomogeneity of the Fe atoms leads to the rich magnetic phase diagram: paramagnetism, ferromagnetism and spin-glass [4].

In this work, we investigate electronic structure, magnetic exchange interaction and T_C of $Ge_{1-x}Mn_x$, and $Ge_{1-x}Fe_x$, by first principles calculations. Our method is based on the Korringa-Kohn-Rostoker (KKR) Green's function method performed by Machikaneyama 2002 package [5]. The randomness of the doped Mn and Fe atoms are considered by the coherent potential approximation (CPA). In order to investigate magnetic property, we calculate the effective magnetic exchange interaction between the transition metals by the Liechtenstein's method based on local force theorem [6]. Moreover, in the case of $Ge_{1-x}Fe_x$, we shed light on the relation between the inhomogeneity of the doped magnetic impurities and magnetic properties, and perform the simulation for the formation process of the nano-structure generated by the spinodal nano-decomposition on the basis of the Monte Carlo simulation. Finally, we estimate the Curie temperature of inhomogeneous system by the random phase approximation (RPA).

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First-principle Design of Low Dimensional Materials for Energy and Spintronic Applications

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Two-dimensional (2D) semiconductors have many unique electronic, optoelectronic, and magnetic properties that is suitable for novel energy related device applications. In this study, using atomic transmutation and global optimization methods, we identified a IV-VI 2D materials, *Pma2*-SiS that can overcome shortcomings encountered in conventional 2D semiconductors [1]. *Pma2*-SiS is found to be both chemically and thermally stable. More importantly, Pma2-SiS has unique electronic, optoelectronic, and thermal properties, including direct bandgaps suitable for solar cells, good mobility for nanoelectronics, low thermal conductivities suitable for thermoelectrics, good property tunability by layer thickness and strain appliance, and good air stability as well. Therefore, Pma2-SiS is expected to be a very promising 2D material in the field of 2D electronics, optoelectronics, and thermoelectrics. Furthermore, we show that half-metallicity (HM) in zigzag graphene nanoribbons (ZGNRs) can be realized by a simple in-plane bending and the induced material has a sizeable HM gap and excellent magnetic stability [3], thus is suitable for low dimensional spintronic applications.

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Frustration-induced spin textures

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Ordering of geometrically frustrated magnets has attracted much recent interest, since it often leads to an unconventional magnetic ordering and novel excitations or "textures" [1]. In this talk, I wish to discuss a variety of multiple-Q states realized in the antiferromagnetic (AF) classical Heisenberg model on the triangular and honeycomb lattices with the nearest- and next-nearest-neighbor (or the third-neighbor) interaction, the J_1-J_2 model or the J_1-J_3 model under applied magnetic fields. In these models, competition between J_1 and J_2 (or J_3) leads to helical spin structures characterized by an incommensurate wavevector. The underlying three-fold crystal symmetry of the lattices then leads to various types of multiple-Q states [2,3].

In the case of the *triangular* Heisenberg model, our Monte Carlo study has revealed several types of multiple-Q states, including single-, double- and triple-Q states. Especially interesting is the triple-Q state, which actually corresponds to the "skyrmion-lattice" state. This skyrmion-lattice state, induced purely by the frustration effect, is "symmetric" in contrast to the standard skyrmion lattice state driven by the anti-symmetric Dzyaloshinskii-Moriya (DM) interaction. It allows both skyrmions (skyrmion lattice) and anti-skyrmions (anti-skyrmion lattice), each characterized by the opposite signs of the scalar chirality. Existence of both skyrmions and anti-skyrmions with opposite topological charges gives rise to the anomalous Hall effect of opposite signs, opening a possibility of a rich variety of transport phenomena. The symmetric nature of skyrmions also leads to a new thermodynamic phase where the skyrmion and the anti-skyrmion lattices form a mixed domain state. Note that neither the anti-skyrmion nor the Z-phase is possible in the standard DM-induced skyrmion-lattice state.

The possible multiple-Q states of the J_1-J_2 *honeycomb* classical Heisenberg model is also investigated [3]. The obtained phase diagram turns out to be quite rich, distinct from that of the triangular model. In contrast to the triangular case, the skyrmion-lattice state is not stabilized. Implications to experiments are discussed.

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Control of Magnetism in Ordered FeRh

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B2-ordered FeRh alloys exhibit fascinating magnetic properties such as antiferromagnetic (AFM)-ferromagnetic (FM) phase transition[1] and AFM memristor functionality[2]. If the magnetic phases of FeRh can further be manipulated by an external means, such controllable magnetic properties will be used in spintronic applications. Here we present our recent work on control of the magnetic phases of FeRh by spin injection and lattice modulation.

Since the magnetic phase of FeRh is stabilized by the subtle balance between the AFM and FM interactions associated with exchange coupling via itinerant electrons, spin accumulation and spin transfer torque effects should play a crucial role, thereby the magnetic phase will be modulated under spin injection condition. In order to inspect spin injection induced magnetic phase transition, local resistivity measurement of FeRh in the vicinity of the Co/FeRh interface was performed[3]. We find that the resistivity of FeRh at 300 K in the AFM phase increases with spin-polarized current density, indicating that partial transition from AFM to FM phases occurs. A discrete feature in I-V characteristics is also seen, which we attribute to possible current induced Barkhausen-type motion of AFM-FM phase boundaries. Modulation of the lattice of FeRh also enables to induce the magnetic phase transition in FeRh since the magnetism arises from strong coupling between spin and lattice as manifested by the lattice expansion at the AFM-FM transition. We study lattice modulation effects on the magnetic phases of FeRh/$BaTiO_3$(100)[4] and show that compressive strain stabilizes the AFM phase across the orthorhombic to rhombohedral structural phase transition of $BaTiO_3$[5]. Electric-field-induced ferroelastic *a*-*c* domain switching of $BaTiO_3$ is also found to induce the FM to AFM phase transition at room temperature. Such an electric field effect can be utilized in spin wave device applications with FeRh[6].

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Multi-scale characterization of polycrystalline thin film PV devices

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Photovoltaics (PV) is becoming an increasingly competitive source of energy with the cost of PV-generated electricity in par with fossil fuel generated electricity in many markets. Currently, PV is dominated by wafer Si, with over 90% of modules manufactured worldwide based on that technology. However, to reach grid parity in more markets, it is widely believed that thin film technologies need to be further developed to be more competitive with wafer Si. Currently, thin film PV devices are based on CuInGaSe2, CdTe and perovskites. All of these thin films tend to have a high density of point and extended defects that deleteriously affect the diffusion length and degrade device properties. This presentation will deal with the characterization of point and extended defects in CuInGaSe2 and CdTe thin films and shed light on longstanding questions.

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Defects in 2D materials

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Atomic scale defects play an important role in modifying the properties of 2D materials. Moreover, these defects influence the characteristics of adatoms, molecules and clusters adsorbed at defect sites regarding electronic, magnetic and optical properties. In this talk, ab initio studies on defects in several 2D materials, e.g., graphene, transition metal dichalcogenides etc. will be discussed. Specifically, theoretical and experimental results on defect-assisted chemical functionalization and gas sensing will be presented.

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Magnetism, spin-lattice-orbital coupling and exchange-correlation energy in oxide heterostructures: Nickelate, titanate, and ruthenate

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Many interesting physical phenomena and material characteristics in transition-metal oxides (TMO) come out of the intriguing interplay between charge, spin, orbital, and lattice degrees of freedom. In the thin film and/or heterointerface form of TMO, this feature can be controlled and thus be utilized. Simultaneously, however, its detailed characteristic is more difficult to be identified experimentally. For this reason, the first-principles-based approach has been playing an important role in this field of research. In this talk, I will try to give an overview of current status of first-principles methodologies especially for the magnetism in the correlated oxide heterostructures or thin films. Nickelate, titanate, and ruthenate will be taken as representative examples to demonstrate the powerfulness of and the challenges to the current methodologies. On the one hand, first-principles calculation provides the useful information, understanding and prediction which can hardly be obtained from other theoretical and experimental techniques. Nickelate-manganite superlattices ($LaNiO_3/LaMnO_3$ and $LaNiO_3/CaMnO_3$) are taken as examples. In this interface, the charge transfer can induce the ferromagnetism and it can be controlled by changing the stacking sequence and number of layers. The exchange-correlation (XC) functional dependence seems to give only quantitatively different answers in this case. On the other hand, for the other issues such as orbital polarization/order coupled with spin order, the limitation of current methodology can be critical. This point will be discussed with the case of tatinate superlattice ($LaTiO_3/LaAlO_3$). For ruthenates ($SrRuO_3$ and Sr_2RuO_4), we found that the probably more fundamental issue could be involved. The unusually strong dependence on the XC functional parametrization is found to give a qualitatively different conclusion for the experimentally relevant parameter regions.

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Materials design toward large perpendicular-magnetocrystalline- anisotropy thin films based on data-science

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Much interest in magnetic tunnel junctions with a perpendicular magnetic easy axis has increased in ultrahigh density and nonvolatile spin-electronics, and efforts for searching promising perpendicular magnetocrystalline anisotropy (MCA) materials have remained a great challenge.[1] However, the effective computational procedure for searching materials with such exciting properties is still lacking due to a difficulty in treating magnetism. Here, in order to show the underlying trends and physics in the magnetism in prototypical multilayer thin-film systems, we carried out first principles calculations by employing six-atomic-layer slabs of three binary systems, Au- Fe, Au-Co, and Fe-Co, on MgO(001) with available different atomic-layer alignments. The magnetic moments for all systems are found to follow the Slater-Pauling rule, i.e., governed by composition of the constituent TMs (the number of valence electrons). In contrast, the MCA energy is found to dramatically depend on the atomic-layer alignments, which varies from 6 meV/atom-area of the MCA energy showing the very large perpendicular MCA to a negative value of -2 meV/atom-area of the in-plane MCA. With an assist of the data-science, we apply compressing sensing for understanding such dispersive MCA and discuss the underlying trends in the magnetism.

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Voltage control of magnetic anisotropy, DMI and exchange interaction in ultrathin ferromagnetic films

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Magnetic anisotropy control using electricfield at room temperature in all solid-state devices was first done using an Fe ultrathin film grown on Au(001) surface and covered by an MgO layer [1]. The effect was soon applied to switch magnetization coherently [2], to excite ferromagnetic resonance (FMR) [3], and to modulate spin waves [4].In this talk, recent progresses in controlling not only magnetic anisotropy (VCMA), but also symmetric/asymmetric exchange interactions in ultrathin ferromagnetic metal films will be shown. Larger VCMA was observed for a system with 1ML Pt insertion between MgO barrier and Fe. In the system, voltage effect to the asymmetric exchange coupling (DMI) was also enhanced. By a numerical simulation, it is shown that the voltage control of DMI allows us to stabilize and destabilize skyrmions in magnetic ultrathin film. Observation of thermally excited spin-wave modes in magnetic tunnel junctions allows us to investigate details of voltage effects in magnetic anisotropy and exchange coupling. Voltage control of VCMA and exchange coupling will be discussed.

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