

Session: Materials for energy and environment (EE)
EE-I01 - EE-I05

EE-I01 (Invited)

CD4⁺ T Cell Counting Using Anti-CD4 Antibody Conjugated Magnetic

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The CD4⁺ T-cell counting device was developed to be used in detection and treatment process of some immunodeficiency diseases, such as HIV, to reduce costs and increase accessibility due to its simplicity and compactness. Magnetic nanoparticles functionalized with carboxyl groups of 100-200 nm in size are conjugated to anti-CD4 antibodies to ensure specific interaction with the CD4 receptor on CD4⁺ T cells. The antibody conjugated magnetic nanoparticles were incubated with 50 μ L of blood sample, then the CD4⁺ T cells were captured by a magnet before being pumped through a microfluidic system with a three-electrode differential capacitance counter. Total CD4⁺ T cells were counted by considering the electrical peaks generated when the cells passed through the electrodes and analyzed using in-built software. The counting results then were compared with the gold standard test of cell counting using the FACS Canto system. The test results show that the developed device gives stable results over a wide range of CD4⁺ T cell concentrations tested (1000–200 CD4⁺ T cells/ μ L blood) and correlates well with the results on the FACS system.

Keywords: CD4⁺ T cell counter, magnetic nanoparticles, microfluidic system

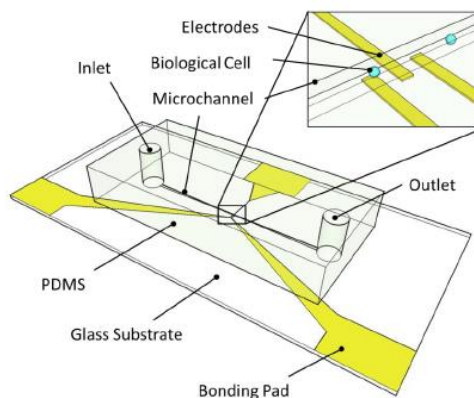


FIG. 1. Schematic design of Microfluidic cell counting system.

EE-I02 (Invited)

Structural analysis of battery materials by atomic-resolution scanning transmission electron microscopy

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The performance of rechargeable batteries is greatly influenced by the microstructure of the electrode materials. However, in many cases, the specific structure-performance relationships are unclear owing to the difficulty of the structural analysis at the atomic scale and nanoscale. Here, we elucidate the microstructures of two kinds of electrode materials by scanning transmission electron microscopy (STEM) and discuss the relationships to the battery performance. The first material is Li_2MnO_3 , a cathode material for Li-ion batteries [1]. The extraction of Li-ions is accompanied by the release of oxygen, Mn/Li cation-mixing, and the introduction of dislocations. These irreversible structural changes could decrease the available number of Li-ions and shorten the cycle life of batteries. The second material is LaNi_5 , a cathode material for fluoride-ion batteries [2]. As shown in FIG. 1, the fluorination reaction in the early stage of the first charging process decomposes LaNi_5 into LaF_3 and Ni nanocrystals, forming nanoscale networks of F⁻-ion- and electron-conducting paths, respectively. This nanoscale network can facilitate the fluorination and defluorination of Ni in the subsequent charge and discharge processes, which increases the practical capacity of batteries.

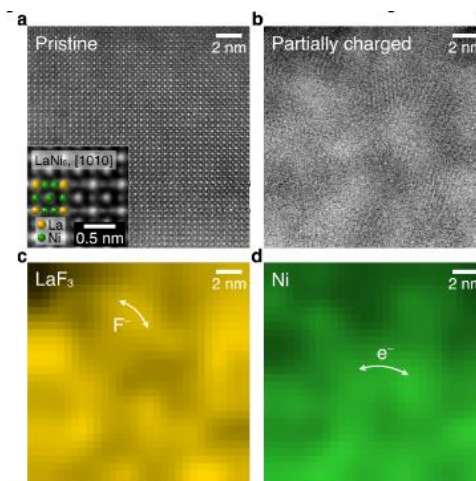


FIG. 1. (a) Annular dark-field (ADF) STEM image of the pristine LaNi_5 sample. (b) ADF STEM image, (c) LaF_3 distribution map, and (d) Ni distribution map obtained from a partially charged sample.

Acknowledgement: This work was supported by the RISING2 (JPNP16001) and RISING3 (JPNP21006) projects from the New Energy and Industrial Technology Development Organization (NEDO), Japan.

Keywords: Scanning transmission electron microscopy, STEM, Battery materials

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EE-I03 (Invited)

Si-based photoelectrodes for water splittingHo Won Jang^{1,*}¹ Department of Materials Science and Engineering, Seoul National University, Seoul, Korea* Corresponding author's email: hwjang@snu.ac.kr; <https://sites.google.com/view/onnl>

The development of a carbon-free hydrogen production method by photoelectrochemical water splitting is a promising pathway to deal with the increased energy demands and deleterious environmental issues derived from the usage of fossil fuels. Silicon, which is the second most earth-abundant element and a small band-gap material, is an applicable candidate for an efficient solar water splitting photoelectrode. However, the stability of Si-based photoelectrode hampers efficient water splitting because of its thermodynamic instability and etching of silicon surface. Until now, much research has been conducted to deal with the challenges of using Si to fabricate efficient and stable photoelectrodes. Over the decades, cheap and earth-abundant transition metal-based electrocatalysts have been investigated. In this presentation, we briefly introduce the photoelectrochemistry and important parameters for evaluating the performance of the Si photoelectrodes. We introduce transition metal-based catalysts, focusing on Ni-, Fe-, Co-, Mo-, W-, and Fe-based oxygen and hydrogen evolving catalysts. Then, we present various strategies to overcome the challenges of silicon by combining the advantages of transition metal-based co-catalysts, which are cost-effective, stable, and highly active for oxygen evolution reaction. Finally, to realize spontaneous water splitting, we introduce Si-based tandem cells combined with transition metal-based materials.

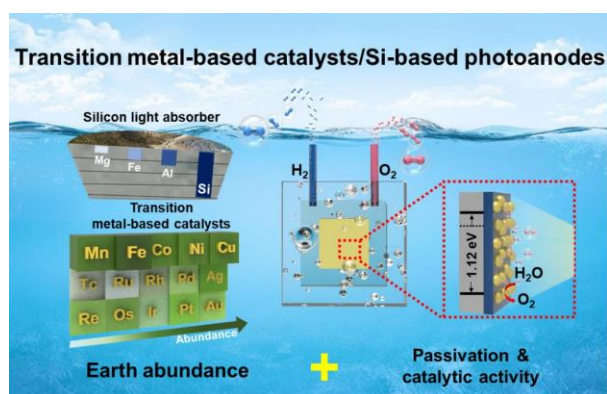


FIG. 1. Si-based photoanodes with cost-effective and high-performance transition-metal catalysts

EE-I04 (Invited)

Defluorination and Adsorption of Tetrafluoroethylene (TFE) on $\text{TiO}_2(110)$ and Cr_3O_3 (0001)

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The capability to join dissimilar materials (cf., e.g., [1-4] and references therein) is a key enabling technology to innovative and sustainable materials design for industrial applications. Some notable examples include polymer-metal composites used in various specialized applications (cf., e.g., [1,2] and references therein). All of these applications fundamentally start with polymer adhesion on metal surfaces. Recently, we report that metal oxide surfaces catalyze the formation of intermediate defluorinated tetrafluoroethylene (TFE) radicals, resulting in enhanced binding on the corresponding metal oxide surfaces [5]. As expected, reactivity of the corresponding metal oxide surfaces depends on the oxygen coordination of metal surface atoms. Thus, introducing oxygen vacancies and non-ionizing radiations to form intermediate radicals could promote binding of polymers to metals and metal-oxide surfaces, allowing for better materials design. This could find significant applications not only in joining dissimilar materials, but also allow for flexibilities in realizing materials with the desired (pre-determined) characteristic properties. Further details will be presented at the meeting.

Keywords: Dissimilar materials, Joining, Metal oxide surface, Catalysis, Materials design

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EE-I05 (Invited)

Single cell capacitance measurement of NIH 3T3 cell using impedance biosensor

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The change of capacitance as a function of time is measured using impedance biosensor for the monitoring of NIH-3T3 cell growth. The capacitance value increased with the growth of NIH-3T3 cell. However, the capacitance behavior showed different tendency between early (from 0 to 140 minutes) and later stage. Therefore, to analyze the difference, we observed the change in the number of cells with real-time images measured using NanoEnTek JuLiTmBr. In addition, the cell counting result was compared with the capacitance measured with various frequencies from 1 kHz upto 800 kHz. As a result, it was confirmed that in the early stage (from 0 to 140 minutes), the cells floating in the medium started to sink to the sensor's surface, and after 140 minutes, cells on the sensor's surface started growth and division. Finally, the average capacitance values of one cell in the early stage and the later stage are presented for each frequency. For example, at 300 kHz, the average capacitance of the cell in the early stage was 0.11 fF, and in the later stage was 0.53 fF. Also, we confirmed that, the measured capacitance increased linearly with the increase of cell numbers, confirming that the parallel arrangement of cells in capacitance measurement.

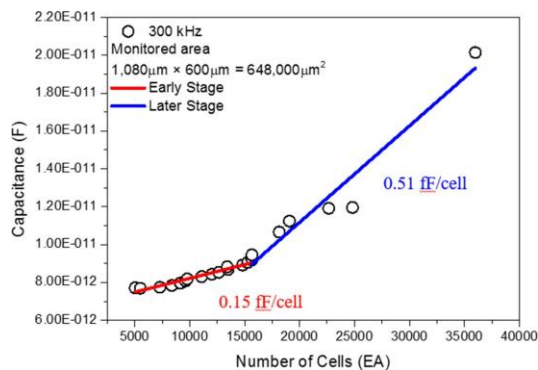


FIG. 1. Graph for comparison with the number of cells and capacitance measured on 300 kHz

Keywords: Impedance biosensor, Capacitance measurement, Single cell capacitance

Session: Multiferroics and magnetic materials (MM)MM-I01 - MM-I11

MM-I01 (Invited)**PbCuTe₂O₆ – a quantum spin liquid candidate showing ferroelectric order close to a quantum critical point**

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PbCuTe₂O₆ has been considered a candidate material for a 3D frustrated quantum spin liquid featuring a highly-connected hyperkagome lattice [1-3]. According to previous magnetic studies, mainly on pressed-powder samples, the system lacks long-range magnetic order down to 0.02 K, and shows diffuse continua in the magnetic spectrum [3] consistent with fractional spinon excitations. There has been an issue relating to the appearance of small anomalies in the powder samples around 1 K of unknown origin [1–3] and signs of a phase transition around this temperature in first-generation single crystals. In this talk, we present results of a comprehensive study of thermodynamic, magnetic and dielectric properties on single crystalline and pressed-powder samples of PbCuTe₂O₆. The low-temperature properties of the powder samples are found to be consistent with the proposed quantum liquid state. Most remarkably, however, an even more exotic behavior is revealed for the single crystals [4], yielding a ferroelectric transition around $T_{\text{FE}} \approx 1$ K [5], accompanied by strong lattice distortions, and a modified magnetic response – still consistent with a quantum spin liquid – but with clear indications for quantum critical behavior [5]. By the application of magnetic fields $B \leq 15$ T, a rich phase diagram is revealed with indications for two field-induced quantum critical points at $B_{c1} \sim 8$ T and $B_{c2} \sim 11$ T.

Keywords: quantum spin liquid, ferroelectricity, quantum criticality

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MM-I02 (Invited)**Application of Magnetic Field for Selective Reaction in Magnetic Alloys**Yoshifuru Mitsui¹ and Keiichi Koyama¹¹ Graduate School of Science and Engineering, Kagoshima University, Kagoshima 890-0065 Japan

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Phase equilibrium and transformation of magnetic alloys can be controlled by magnetic field [1] because of the gain of Zeeman energy to the ferromagnetic phases. We have investigated that magnetic field also influenced the solid-solid [2], solid-liquid [3,4], and gas-solid reaction [5]. For example, solid-phase reactive sintering of ferromagnetic MnBi from non-ferromagnetic Mn and Bi particles was enhanced by magnetic field and obtained MnBi phase was uniaxially-oriented [2]. Above in-magnetic-field synthesis indicated the possibility of selective reaction of the ferromagnetic phase from non-ferromagnetic precursor or raw materials. In diffusion couples, the reacted phases with various magnetic state exhibited. Therefore, it is expected that the in-magnetic-field reaction using diffusion couples show the unique phase growth. Recently, we investigated the effects of magnetic field on the solid-liquid reactions of diffusion couples between magnetic metal and low melting-point metal. In this study, in-magnetic-field reactions of ferromagnetic Fe-Ga [3], and non-ferromagnetic Mn-Ga [4] were investigated.

In Fe-Ga diffusion couple, Fe₃Ga, the eutectic regions of Fe₃Ga and Fe₆Ga₅, Fe₆Ga₅, Fe₃Ga₄ and FeGa₃ phase were observed at Fe/Ga boundary. The growth rate of reacted phase was suppressed by magnetic field at both ferromagnetic and paramagnetic state of α -Fe. It was found that magnetic-field-induced reduction of the growth rate was due to the pre-exponential factor of the diffusion coefficient, and the activation energy did not change. On the other hand, in Mn-Ga diffusion couple, many phases with various magnetic state exhibited at Mn/Ga boundary as reacted phase. Mn-rich phases were ferrimagnetic or ferromagnetic, and Ga-rich phases were non-ferromagnetic. The phase growth of Ga-rich phases was faster than that of Mn-rich phases in a zero field. Meanwhile, the growth rate for Mn-rich phase did not change in 5 T, but the growth rate for Ga-rich phase reduced. Therefore, it is indicated that magnetic field promotes the selective growth of ferromagnetic/ferrimagnetic phase.

Keywords: ferromagnetic alloys, high magnetic field, reaction**References**

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MM-I03 (Invited)

Crystal structures and electronic properties of vanadium oxides

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Vanadium shows valence states ranging from 2+ to 5+. The charge, orbital, and spin degrees of freedom of vanadium ions lead to a variety of physical properties and functions. In this study, we especially focus on perovskite-type and ilmenite-type oxides containing tetravalent vanadium ions. Tetravalent vanadium ion has only one t_{2g} electron, which causes the Jahn-Teller effect and the formation of molecular orbitals between adjacent vanadium ions. By utilizing these effects, we found novel properties and functions, such as colossal negative thermal expansion in electron-doped PbVO_3 [1,2], and cation dimerization in the ilmenite-type vanadium oxides $M\text{VO}_3$ (M = divalent metal ions) [3-5], as shown in FIG 1.

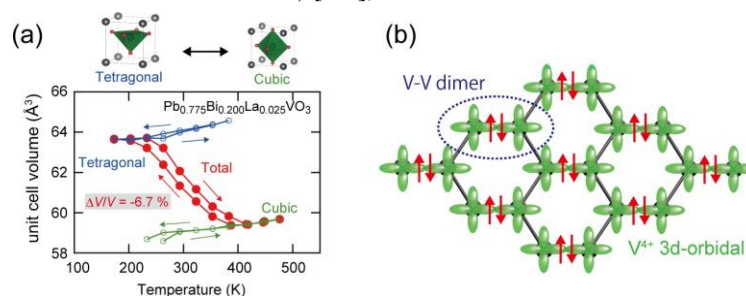


FIG. 1. (a) Colossal negative thermal expansion in electron-doped (perovskite-type) PbVO_3 . (b) Schematic of cation dimerization in ilmenite-type MgVO_3 .

Keywords: Strongly correlated electron systems, High-pressure synthesis, Oxides, Magnetism, Structure transition

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MM-I04 (Invited) (FREE)

Title

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Abstract.

FIG. 1. [1]

Keywords: key1, key2, key3, key4

References

[1] ref1

MM-I05 (Invited)

Tuning the Ground State of Strongly correlated $\text{EuPd}_2(\text{Si}_{1-x}\text{Ge}_x)_2$ using He-Gas Pressure

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The strongly correlated intermetallic compound EuPd_2Si_2 is one of the rare examples where a strong valence-change crossover is observed as a function of temperature. The valence change from $\text{Eu}^{(2+\delta)^+}$ to $\text{Eu}^{(3-\delta')^+}$ which occurs in a small temperature range is accompanied by pronounced lattice effects together with significant changes in the magnetic properties [1]. According to spectroscopic and thermodynamic measurements, this material is located on the high-pressure side (crossover range) of the second-order critical endpoint (CEP). This end point terminates the first-order valence transition line in the generalized p - T phase diagram of Eu-based intermetallics [2]. At the CEP novel collective phenomena which originate from a particularly strong coupling between electronic-, magnetic- and lattice degrees of freedom can be expected [3]. The aim of our study is to identify a suitable chemical modification of EuPd_2Si_2 , corresponding to a negative chemical pressure, so that the CEP can be accessed via fine pressure tuning by using He-gas technique.

We present magnetic susceptibility measurements and thermal expansion data taken on high-quality single crystals of $\text{EuPd}_2(\text{Si}_{1-x}\text{Ge}_x)_2$ for nominal Ge-concentrations $0 \leq x_{\text{nom}} \leq 0.2$ in the temperature range $2 \text{ K} \leq T \leq 300 \text{ K}$. The experiments have been performed using He-gas pressure up to 0.5 GPa. For $x = 0$ at ambient pressure we observe a pronounced valence crossover centered around $T_V \sim 160 \text{ K}$ leading to a non-magnetic ground state. This valence-change crossover is characterized by an extraordinarily strong pressure dependence of $dT_V/dp \approx (80 \pm 10) \text{ K/GPa}$. As expected, T_V shifts to lower temperatures with increasing Ge-concentration, reaching $T_V \sim 90 \text{ K}$ for $x_{\text{nom}} = 0.1$, while still showing a non-magnetic ground state. In contrast, for the system with $x_{\text{nom}} = 0.2$ we observe a magnetic ground state with long-range antiferromagnetic order setting in below $T_N = 47.5 \text{ K}$. The important finding is that the application of weak pressure as low as 0.2 GPa the long-range magnetic order can be suppressed giving way to a non-magnetic ground state with pronounced valence fluctuations. We therefore consider this compound a promising target material for studying pressure-induced strong-coupling effects.

Keywords: strongly correlated materials, valence transition, He-gas pressure

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MM-I06 (Invited)**Soft Magnetic Fe(Co)-based High Bs Nanocrystalline Alloys for Applications at Elevated Temperatures**Ivan Škorvánek^{1,*}, Branislav Kunca¹, Jozef Marcin¹, Peter Švec²¹ Institute of Experimental Physics, Slovak Academy of Sciences, 040 01 Košice, Slovakia² Institute of Physics, Slovak Academy of Sciences, 842 28 Bratislava, Slovakia

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The continuing interest in Fe(Co)-based nanocrystalline alloys is motivated mainly due to the combination of high saturation magnetic flux density with good magnetic softness and their capability to operate at elevated temperatures. A further improvement of magnetic performance in these alloys is possible by using a careful compositional tuning as well as by employing special processing techniques resulting in optimal phase content and reduced grain sizes. Special attention of our work is focused on rapid annealing technique that utilizes a compression of samples between pair of pre-heated Cu blocks [1]. Here, very high heating rates and short processing times result in a formation of markedly smaller nanocrystalline grains as compared to conventional furnace annealing. Selected results showing the impact of rapid annealing on the soft magnetic properties will be presented for high Bs Fe-(Co)-B-(Cu) and Fe-Sn-B alloys with a reduced metalloid content. A part of our research interest is devoted also to the application of external magnetic field during the conventional furnace annealing in order to improve their soft magnetic characteristics. It is shown that the specimens of Fe-Co-B-(Cu) amorphous and nanocrystalline alloys annealed in conventional furnace without a presence of external magnetic field exhibit an unwanted increase of coercivity. In addition, the corresponding hysteresis loops show a presence of steps due to the depinning of domain walls from the positions stabilized during annealing. After heat treatment in longitudinal or transverse magnetic field one can obtain smooth hysteresis loops with markedly reduced coercivity. We show that similar effects can be achieved also by employing of rapid annealing techniques. Examples of our work on testing the magnetic behavior of these alloys at elevated temperatures [2] will be briefly presented and discussed.

Keywords: nanocrystalline alloys, heat treatment, microstructure, magnetic properties**Acknowledgement:** This work was supported by the projects APVV-19-0369 and VEGA 2/0171/19**References**

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MM-I07 (Invited)

X-ray Spectro- and Microscopic-Techniques on Novel Materials

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The presentation will focus on the use of synchrotron radiation-based spectroscopic and microscopic techniques for probing the electronic and atomic structures of novel and low dimensional materials. Elucidating electronic structures during an electrochemical reaction of energy materials, such as batteries and electrochemical materials, is essential to understanding better the energy conversion mechanism. Unlike other techniques, *in-situ* X-ray absorption spectroscopy (XAS) directly provides information on electronic structures, which is critical for tracking the charge states of active elements during a chemical reaction. The studies primarily have been involved with using XAS, X-ray emission spectroscopy (XES)/resonance inelastic X-ray scattering (RIXS) at Taiwan Photon Source (TPS)/Taiwan Light Source (TLS) and other synchrotron-related facilities. This presentation will report the current achievements and perspectives of XAS, XES/RIXS and Scanning Transmission X-ray Microscopy (STXM) techniques on relevant materials. Emerging characterization tool developed at TPS 45A and 27A beamlines will be also presented.

Keywords: XAS, XES/RIXS and STXM

MM-I08 (Invited)

Substrate Polarity, Phase Stability, Electronic Structure and Magnetic Properties of Multiferroic YMnO_3 Thin Films

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In this study, we explored the effects of surface polarity and orientation of substrates on the phase stabilisation of multiferroic hexagonal YMnO_3 (YMO) thin films. It is found that the configuration of the initial atomic layers during the growth of YMO thin films plays a key role in minimising the misfit strain and, hence, stabilising the resultant phases. Remarkably, it is also observed that the polarity of the terminating substrate surface is playing an equally important role in determining the eventual microstructure, electronic structure and magnetic properties of the YMO films. We suggest that the extent of charge accumulation induced by the substrate surface polarity may have resulted in significant effect on the film/substrate interfacial intermixing, which, in turn, alters the crystalline structure and, hence, physical properties of the films. Results obtained from YMO films grown on $\text{MgO}(100)$ and $\text{MgO}(111)$ substrates will be presented and discussed. It is believed that the present results represent an alternative possibility of manipulating the magnetic properties of YMO films via interfacial engineering, which might be beneficial for various next-generation oxide electronics.

Keywords: Surface Polarity of Substrate, Phase stabilisation, Multiferroic manganites thin films, Electronic Structure, Magnetic properties

MM-I09 (Invited)

Point Contact Andreev Reflection Spectroscopy on Topological Kondo Insulator SmB₆

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SmB₆ is famous for Kondo insulator (KI). In KI, the electrical resistivity increases rapidly below the Kondo temperature due to the formation of hybridization gap near the Fermi energy, which originates from the hybridization between the conduction electrons and *f* electrons (*c-f* hybridization). Meanwhile, the electrical resistivity of SmB₆ saturates below $T \sim 5$ K despite the full development of the hybridization gap, which has been interpreted as the existence of the in-gap state inside the hybridization gap [1]. On the other hand, recently, a new scenario is proposed by Dzero *et al.*, which pointed out that SmB₆ is classified as a topological Kondo insulator (TKI) [2]. If the SmB₆ is a TKI, the metallic state exists on a surface of SmB₆. So far, to explore the surface metallic state on SmB₆, many experiments have been conducted [3]. However, the origin of the metallic behavior at low temperatures is still controversial. In the present study, we performed point contact Andreev reflection spectroscopy (PCARS) measurements to examine the metallic surface state of SmB₆.

Figure 1 shows the PCARS spectrum of SmB₆ using a Nb probe tip at $T = 4.5$ K, where the temperature is lower than the superconducting transition temperature T_c of Nb. A narrow dip structure is observed at around zero bias, which is overlapped by a broad asymmetric dip-shaped background. Importantly, the narrow dip structure disappears above the T_c of Nb, indicating that the narrow dip comes from the Andreev reflection at SmB₆/Nb interface. These demonstrate the existence of the surface metallic state on SmB₆. From the fitting of spectra by the theoretical model, the spin polarization of the surface state is estimated to be $P \sim 0.5$, strongly suggesting that a high spin polarized metallic state exists on the surface although SmB₆ is a paramagnetic insulator. Our findings support that SmB₆ is a topological Kondo insulator.

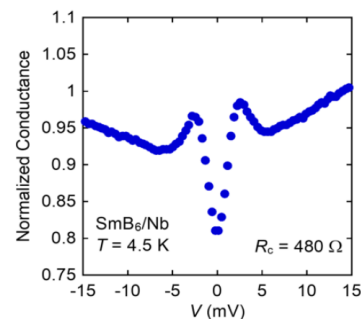


FIG. 1. dI/dV spectra of SmB₆/Nb interface at $T = 4.5$ K.

Keywords: topological Kondo insulator, SmB₆, point contact Andreev reflection

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MM-I10 (Invited)

Searching for the origin of magnetic inhomogeneity of FeRh film

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Antiferromagnetic (AFM) FeRh exhibits magnetic phase transition from AFM to ferromagnetic (FM) system around room temperature. Therefore, utilizing the phase transition characteristics in modern spintronic applications get more attention due to advantageous AFM characteristics. In order to adapt device architecture, the interface characteristics of FeRh film are essential. Previously, it has been known that the pristine FeRh films exhibit residual ferromagnetism in the AFM state (i.e., below transition temperature). Therefore, it is disadvantageous to obtain magnetically clean interfaces owing to the formation of residual ferromagnetism at the interfaces. In this presentation, we examined the temperature- and depth-dependent magnetic properties of DC sputtered FeRh films to enhance our understanding of the residual ferromagnetism in the AFM state. As a result, we found the presence of non-uniform magnetic properties at the interfaces. Furthermore, we showed the different origins of residual ferromagnetism at the top and bottom interfaces.

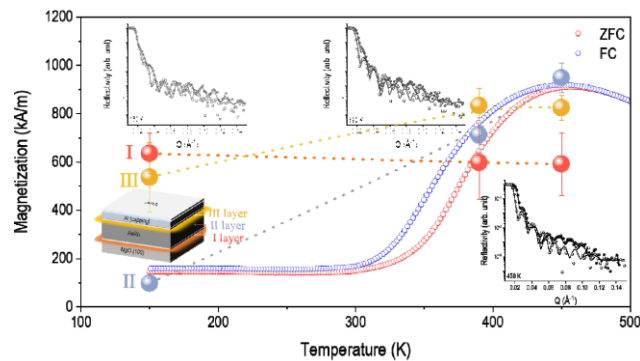


FIG. 1. Temperature- and depth-dependent magnetic characteristics of FeRh film

Acknowledgement: This study was supported in part by NRF-2018R1D1A1B07045663, NRF-2020K1A3A7A09077715, NRF-2021M3H4A6A02045432, NRF-2022M3H4A1A04071154, and No. 2021R1A6C101A429.

MM-I11 (Invited)**Magnetic Skyrmion for the Brownian computing**

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Magnetic Skyrmion is a particle-like magnetic excitation in ferromagnetic material. The magnetic Skyrmion shows Brownian motion [1, 2] as if it is a micro- or nano-size particle sintered in a liquid. The skyrmion system can be an ideal platform for designing stochastic computer [1] and/or Brownian computer [3].

To create the Skyrmions, Ta/Co-Fe-B /Ta sandwiched films [4] possessing perpendicular magnetic anisotropy and the interfacial-Dzyaloshinskii-Moriya interaction (i-DMI) were fabricated. Changing the upper and lower Ta film thicknesses independently, the ratio of the i-DMI energy to the magnetic anisotropy energy was adjusted. In addition, by eliminating the annealing process, the generation of grain boundaries was suppressed. The annealing free process enhanced the diffusion coefficient of skyrmions by a factor of more than 10 compared to the previous study [1] and comparable to the recent observations [4, 5]. The Skyrmions are adjusted to have a diameter of about 1 μm to allow the observation by an optical microscope with polarization analysis (MOKE microscope).

In this talk, film preparation and microfabrication of skyrmion channels and boxes [6] by means of SiO₂ add layer deposition [4] and ion implantation [7] will be introduced. In the end, the perspective on the implementation of the Brownian computer will be discussed.

Acknowledgments: This work was supported by the ULVAC, JSPS Grant-in-Aid for Scientific Research (S) Grant Number JP20H05666, Japan, CREST (Non-classical Spin project, JPMJCR20C1) of the Japan Science and Technology Agency, and Center for Spintronics Research Network (CSRN), Graduate School of Engineering Science, Osaka University.

Keywords: Skyrmion, Brownian computer, Spintronics, Diffusion, Artificial intelligence

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Session: Photonics and Hybrid Materials
PH-I01 - PH-I06

PH-I01 (Invited)**Local environment of emission center ions in phosphor materials**Tomoyuki Yamamoto^{1,*}¹ Waseda University, Shinjuku, Tokyo, 169-8555, Japan

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Recently importance of the phosphor materials is raising in many fields, since the applications of the phosphor materials are not only for our ambient lightings but also for agriculture and generations of electricity together with solar cells. Most of the phosphor materials are synthesized with doping techniques, i.e., incorporation of dilute ions as emission center. For instance, rare-earth ions such as Pr and Eu ions are often doped in wide-gap host materials such as oxides and fluorides, which act as an emission center for the efficient phosphors. It is well known that photon emission intensity of the phosphor materials are strongly related to the local environment of emission center ions.

In this presentation, local environment analysis of Mn ions in red phosphors both with experimental and theoretical methods will be introduced. For the former experimental analysis, X-ray absorption near edge structure (XANES) and electron spin resonance (ESR) analysis for Mn ions are shown, while for the latter theoretical one the first principles calculations within a framework of the density functional theory (DFT) level are shown. In some cases, co-doping can enhance the emission intensity of the phosphors. To reveal the reason why such enhancement occurs due to co-dopings, combined analysis of the above experimental and theoretical calculations were carried out for $\text{CaAl}_2\text{O}_9:\text{Mn}$ co-doped with divalent ions, such as Mg^{2+} , Zn^{2+} , Cd^{2+} and Sr^{2+} [1], which suggested co-doped ions contribute to the change in local environment of Mn ions.

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PH-I02 (Invited)**Luminescence and non-linear optical properties at mid-infrared spectral range**

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The Mid-red (MIR) spectral range shown great important for both fundamental and possible applications such as optical communications, gasses pollutants detection, trace chemical analysis as well as the next generation imaging devices for remote sensing and medical contrast agents due their fundamental absorption features in the wavelength regions from 1,5 μm to 15 μm . Therefore, strong emitting sources in MIR spectral range will be extremely useful in the construction of lidar allowing remote detection of gases (including hazardous gases), which is important for health and environmental protection, chemical rescue, the mining industry or military applications. Currently, the most effective ways of obtaining radiation in MIR are luminescence phenomena or radian form CO₂ lasers by utilise a non-linear-optical effects (SHG, THG).

From the other hand, the range of high spectral transparency for chalcogenide or halide crystals, glasses or ceramics (from about 400-700 nm to several dozen micrometres) is unique and do not available for oxygen containing materials. In addition, these materials with low energy of the phonon system are predestined at the matrices for embedding active elements (RE or 3d elements) for long-wave luminescence or construction lasers operating in the mid-infrared range along with explanation limitations regarding embedding of rare earth ions in chalcogenide/halide structures, which is not an easy experimental undertaking.

Next, we focus on the influence of the structural properties (composition, complexity and defects, presenting in real materials) on the stability, luminescence optical and nonlinear-optical efficiency for the group of binary, ternary and quaternary halide and chalcogenide crystals, that have found practical applications in IR optoelectronics. Especially above-mentioned defects shown the significant impact on nonlinear-optical and luminescence properties.

Keywords: Mid-Red, luminescence, non-linear optics, halides, chalcogenides

PH-I03 (Invited)

Magnetoplasmonic core-shell nanowires: synthesis and self-assembly for structural colors and chiral metasurfaces

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A facile one-pot solvothermal synthesis method was developed for growing an anisotropic hybrid nanostructure composed of magnetic oxide nanoparticles coated on plasmonic gold nanowires (Au@Fe_xO_y MagPlas NWs). The effects of reaction temperature, time, reducing agent and precursor as well as post-synthesis treatment were optimized to produce highly uniform NWs in the aspect ratio of 25 ~ 82. The synthesized structures inherited the magnetic properties from the iron oxide layer and anisotropic localized surface plasmon resonance (LSPR) of the gold nanowires, which are potentially useful for a wide range of optical and sensing applications. Especially, by exploiting the interaction of NWs with an external magnetic field, MagPlas NWs were aligned into 2D photonic surfaces with high periodicity, which can generate distinctive structural colors that are uniquely iridescent and polarization-sensitive. Furthermore, we demonstrated the fabrication of a bioinspired Bouligand-type chiral cholesteric metasurface, by stacking the 2D aligned microchains continuously with a rotating pitch angle. This film displays remarkable sensing capability with circular dichroism spectroscopy, which could detect the change of surface alignments upon the addition of analyte molecules. These intriguing properties of MagPlas anisotropic NWs and their self-assemblies could be consequently valuable for developing photonic, catalysts, and sensing applications.

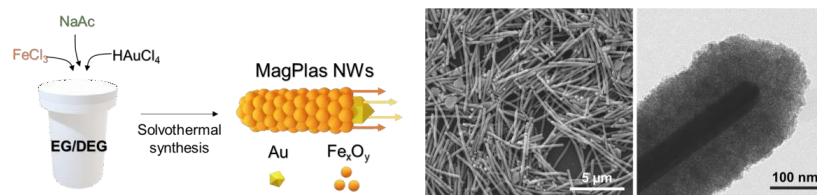


FIG. 1. Schematics of the synthesis process and electron microscopic images of the synthesized MagPlas NWs

Keywords: magnetoplasmonic, nanosynthesis, nanowires, chiral, structural color

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PH-I04 (Invited)

High-performance Colorful Semitransparent Organic Solar Cells with Etalon Electrodes

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Semitransparent organic solar cells (STOSCs) are a technology that combines the benefits of visible light transparency and light-to-electrical energy conversion. One of the greatest opportunities for STOSCs is their integration into windows and skylights in energy-sustainable buildings. For this application, the aesthetic aspects of solar cells may be as important as their electrical performance. Here, our strategy enables to achieve high-quality and colorful STOSCs using Fabry-Pérot etalon-type electrodes. These electrodes are composed of an antimony oxide (Sb_2O_3) cavity layer and two thin Ag mirrors. These dichroic tri-layer structures perform two functions as top conducting electrodes and color filters. These dual-function electrodes were applied to photovoltaic devices and displayed vivid colors, natural transparency, and good performance as compared to devices that use conventional metal electrodes. Furthermore, to achieve saturated colors and low photocurrent losses, active layer materials were selected such that their transmittance peaks matched the transmittance maxima of the electrodes. These strategies for colorful STOSCs result in power conversion efficiencies (PCEs) of up to 13.3% and maximum transmittances (T_{MAX}) of 24.6% in blue devices, PCEs of up to 9.71% and T_{MAX} of 35.4% in green devices, and PCEs of up to 7.63% and T_{MAX} of 34.7% in red devices.

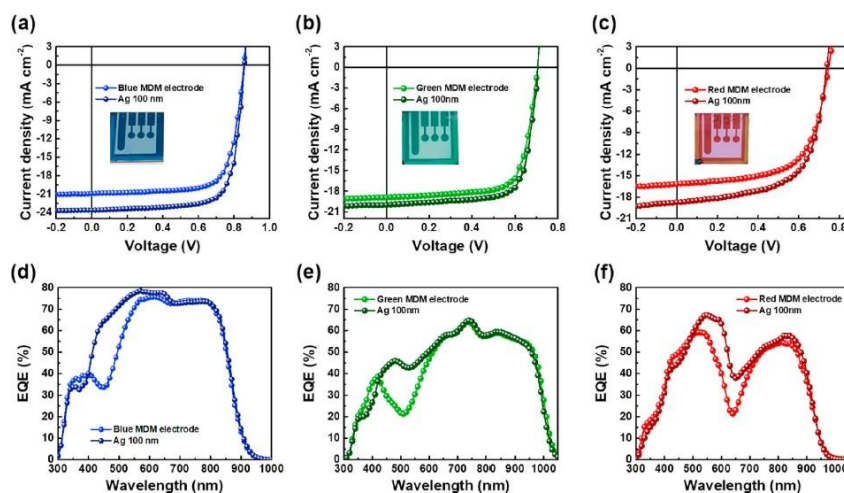


FIG. J-V curves and EQE spectra of the control (Ag 100 nm) and semitransparent (blue, green, red MDM electrodes) devices based on (a, d) PM6:Y6 as blue active materials, (b, e) PTB7-Th:CO₂:8DFIC:PC₇₁BM as green active materials, (c, f) J52:IEICO-4F:NIDCS-HO as red active materials, respectively, under AM1.5G (100 mW cm⁻²) illumination.

Keywords: organic solar cells, colourful, semitransparent, antimony oxide, Fabry-Pérot etalon

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PH-I05 (Invited)

Probing the Exciton Wavefunction in Low-Dimensional Materials by Photoemission Momentum Microscopy

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The strong and long-lived excitonic response of low-dimensional semiconductors such as two-dimensional transition metal dichalcogenides (TMDs) and zero-dimensional organic semiconductors provides an outstanding opportunity for innovation, with applications ranging from organic solar cells to new logic devices beyond current electronics. Efficient application of these materials, however, depends on an accurate understanding of the opto-electronic response, ultimately characterized by a complete knowledge of the out-of-equilibrium wavefunction that arises upon optical excitation. Such knowledge, which is extremely difficult to achieve using experimental and theoretical methods alike, has now come within our grasp through the development of multi-dimensional time- and angle-resolved photoelectron spectroscopy devices [1]. In particular, this has enabled 1) a fully time-, 2D momentum-, energy-resolved characterization of the out-of-equilibrium electronic structure and 2) the application of photoemission orbital tomography to acquire direct access to the real-space properties of the electronic wavefunction in thin organic molecular layers [2]. As demonstrated recently [3], this does provide a unique access to the real-space excited-state wavefunction under optical excitation. Here, I will demonstrate how time-resolved momentum microscopy allows us to trace the formation of interlayer excitons in a twisted TMD heterostructure through space and time [4], and secondly enables the characterization of out-of-equilibrium excitonic wavefunctions in a crystalline buckminsterfullerene (C_{60}) multilayer.

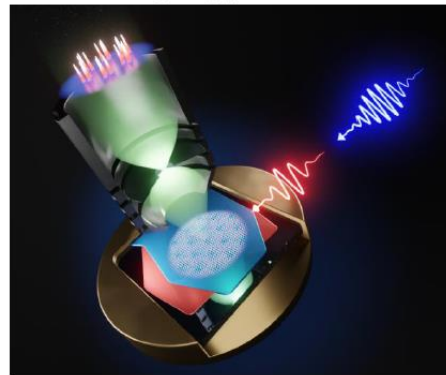


Fig. 1: Photoemission momentum microscopy enables to probe the full energy- and 2D momentum-resolved electronic structure with femtosecond time resolution, and provides unprecedented information on dynamics in micron-scale TMD heterostructures, organized organic thin films and many other low-dimensional systems.

Keywords: Excitons, ARPES, photo-emission orbital tomography, pump-probe

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PH-I06 (Invited)

Metamaterials: Plasmonic properties, ultrafast dynamics, heat transfer, and tuneability

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In macroscopic physics, many properties of bulk materials are usually independent of the sample size. Metamaterials that are made up by periodic subwavelength pieces of matter, however, reveals a not only different but also fascinating picture: their properties are not derived from the constituent materials, but from their newly designed structures [1]. The motivation behind metamaterial research in our group arises, on one hand, from fundamental interest in various aspects of physical properties from the nano-scale to the solid-state limit, and on the other hand, from the desire of using smarter structures for novel technological applications. In this talk, we present our results on plasmonic properties, ultrafast dynamics, heat transfer, and tuneability of metamaterials (see Fig. 1) operating at various frequency regimes (GHz, THz, and optics) [2,3]. The recent implementation of metamaterials for energy harvesting and advanced sensing applications is also discussed [4].

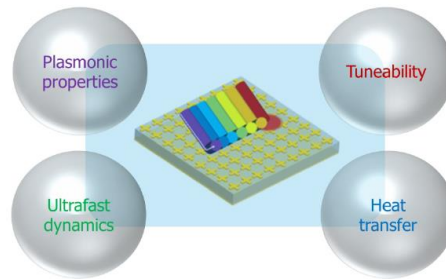


FIG. 1. The motivation behind metamaterial research arises from fundamental interest in various aspects of physical properties, for example, plasmonic properties, ultrafast dynamics, heat transfer, and tuneability.

Keywords: metamaterials, sensing, plasmonics, ultrafast dynamics, tuneability

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Session: Spintronic materials and devices
SD-I01 - SD-I12

SD-I01 (Invited)

Observation of flat band in millimeter-scale magic-angle twisted bilayer graphene

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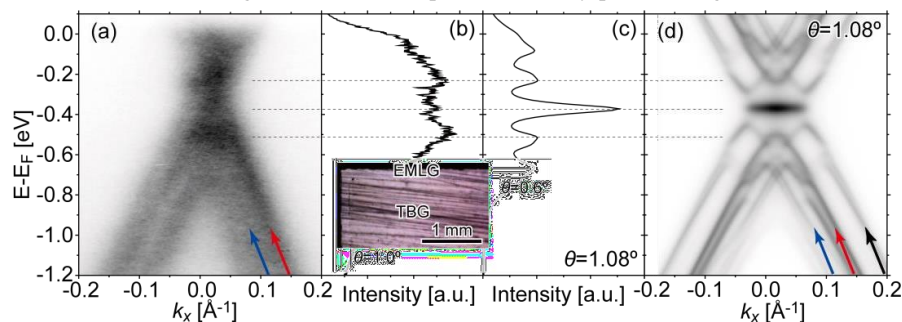
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Twisted bilayer graphene (TBG) has attracting great interest as a method to introduce a novel degree of freedom in the electronic states in graphene. Particularly, the magic-angle (1.1°) TBG exhibited superconductivity, induced by the flat band [1]. In order to expand the field of “twistronics”, the large-area TBG formation and the control of the flat band energy are required. In this study, we obtained the $5 \times 5 \text{ mm}^2$ TBG sample, and observed the electronic structure, including the flat band. We obtained two samples of epitaxial monolayer graphene (EMLG) by thermal decomposition of SiC. We exfoliated one graphene from the SiC substrate, and transferred it onto other EMLG/SiC with a twist angle [2]. Angle-resolved photoemission spectroscopy (ARPES) was carried out to reveal the electronic structure of the TBG samples.

Figure 1 is the ARPES results of a TBG sample [3]. In this TBG sample, EMLG of $5 \times 5 \text{ mm}^2$ size was transferred with a target twist angle of 1.1° , and its optical micrograph is shown in the inset. The ARPES image in (a) includes two or more bands as shown by blue and red arrows. One of the striking features of the ARPES image is the high density of states at -0.22 and -0.51 eV. In addition to the states at -0.22 and -0.51 eV, another band at -0.37 eV was observed in between them, as shown by dotted lines in the figure. These features can be readily explained by the calculated spectral function shown in Fig. 1(c) and (d), which clearly shows the flat band at -0.37 eV.

FIG. 1. (a) ARPES image of the TBG sample. (b) Intensity profile along $k_x = 0.016 \text{ \AA}^{-1}$ line



in (a). (c)(d) Spectral function of 1.08° TBG. (c) Intensity profile along $k_x = 0.016 \text{ \AA}^{-1}$ line in (d).

Keywords: graphene, twisted bilayer graphene, magic-angle, flat band, ARPES

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SD-I02 (Invited)**Towards Magnetic Skyrmionics**Chanyong Hwang^{1,*}¹ Quantum Technology Institute, Korea Research Institute of Standards and Science, Daejeon, 34113, Korea

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Magnetic skyrmion has drawn lots of attention due to its topological characteristics and its use as an information carrier. Over the last decades, the formation of the magnetic skyrmion was quite limited to few cases, where kinds of perturbative methods have been applied. Since this formation process is not quite systematic, the sample is quite limited. We have found the systematic way to form, delete and move the magnetic skyrmion in all kinds of magnetic films with perpendicular magnetic anisotropy. With this general recipe for skyrmion formation, we can drive lots of devices which can be used in spintronics. Skyrmion racetrack memory, magnetic skyrmion transistor, also neuromorphic device with magnetic skyrmion will be presented.

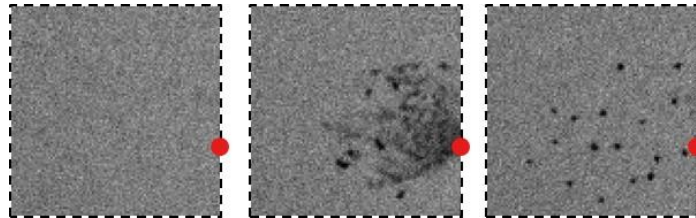


FIG. 1. Formation of Magnetic Skyrmion using vertical current pulse

Keywords: magnetic skyrmion, PMA, skyrmionics, spintronic device**References**

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SD-I03 (Invited)

Neuromorphic devices based on electrochemical metallization and charge trapping

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Neuromorphic systems have attracted much attention because they can provide suitable solutions for problems emerging in ‘big data’ era. Up to now, neuromorphic systems emulating the functions of human brain have been implemented in a variety of applications but have revealed limitations due to a large number of devices and high energy consumption. Therefore, it is required to develop neuromorphic systems based on neuromorphic devices which emulate the hardware of human biological systems, such as synapses and neurons.

In this talk, I will introduce recent research activities of my laboratory to implement neuromorphic devices based on inorganic nano materials. By combining cation migration and ferroelectric polarization reversal, we implemented an energy efficient and selectively activated synaptic device [1]. It was found that electrochemical metallization devices with a ferroelectric electrolyte could implement both neuron and synaptic devices depending on the active electrode material. Progressive and stable synaptic plasticity with femtojoule energy consumption could be achieved by the interface engineering of a metal/ferroelectric/semiconductor [2]. Multi-stable resistive states and synaptic behaviors were observed in a capacitor structure with an emerging two-dimensional insulator, CrPS4 [3]. It was demonstrated that vertical Ag/CrPS4/Au capacitors could be promising inorganic devices compatible with next-generation, flexible neuromorphic technology [4]. Furthermore, a vertical two-terminal Pt/bi-layer Sr_{1.8}Ag_{0.2}Nb₃O₁₀ nanosheet/Nb:SrTiO₃ device could emulate heterosynaptic plasticity by controlling the number of electron trap sites through A-site deficiency control of the nanosheet.

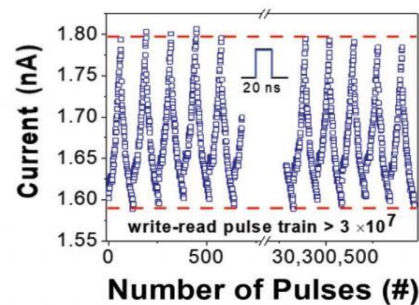


FIG. 1. Demonstration of stable synaptic weight update for $i/\text{Pb}(\text{Zr}_{0.52}\text{Ti}_{0.48})\text{O}_3/0.5$ wt.% Nb-doped SrTiO_3 with ultralow energy consumption below 9 fJ during over 3×10^7 pulses.

Keywords: neuromorphic, synaptic device, neuron device, ferroelectric, heterosynaptic plasticity

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SD-I04 (Invited)

Superconducting Diode Effect in Rashba Superlattice

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The diode effect is fundamental to electronic devices and is widely used in rectifiers and AC-DC converters. However, conventional diodes have an energy loss due to finite resistance. We found the superconducting diode effect (SDE) in Nb/V/Ta superlattices with a polar structure, which is the ultimate diode effect exhibiting a superconducting state in one direction and a normal state in the other [1-3]. SDE can be considered as the nonreciprocity of the critical current for the metal-superconductor transition. We also found the reverse effect, i.e., the nonreciprocal critical magnetic field under the application of the supercurrent [4]. We also found that the polarity of the superconducting diode shows a sign reversal as a magnetic field is increased, which can be considered as the crossover and phase transitions of the finite-momentum pairing states predicted theoretically [5]. SDE in Nb/V/Ta superlattices needs an application of an external magnetic field to break the time reversal symmetry, which is a disadvantage in applications. We recently succeeded in demonstrating SDE in a zero-field by introducing ferromagnetic layers in superlattices. The polarity of the SDE is controlled by the magnetization direction of the ferromagnetic layer, leading to development of novel non-volatile memories and logic circuits with ultralow power consumption.

Acknowledgement: This work was partly supported by JSPS KAKENHI Grant Numbers (18H04225, 18H01178, 18H05227, 20H05665, 20H05159, 21K18145), the Cooperative Research Project Program of the Research Institute of Electrical Communication, Tohoku University, the Collaborative Research Program of the Institute for Chemical Research, Kyoto University, and the Russian Ministry of Science and Higher Education under Megagrant No. 075-15-2021-607.

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SD-I05 (Invited)

Enhanced Anomalous Nernst Effect in Metallic SuperlatticesTakeshi SEKI^{1,*}¹ Institute for Materials Research, Tohoku University, Sendai, 980-8577, Japan

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Spin caloritronics, the field studying the interconversion between charge current (J_c) and heat current (J_q) mediated by spin current (J_s) and/or magnetization (M), has attracted much attention not only for academic interests but also for practical applications. The newly discovered spin caloritronic phenomena have stimulated the renewed interest in the thermoelectric phenomena in ferromagnets. One of the thermoelectric phenomena in ferromagnets is the anomalous Nernst effect (ANE), in which J_c appears in the cross-product direction of M and a temperature gradient (∇T). Although ANE has been known for a long time, the microscopic physical picture for ANE has not fully been understood. In addition to the fundamental point of view, this magneto-thermoelectric effect is possibly beneficial for thermoelectric conversion applications. The key for the ANE-based thermoelectric conversion is to find a material with a large anomalous Nernst coefficient (S^{ANE}).

We previously reported the enhancement of ANE in the Fe-based metallic multilayers [1], implying that the low dimensionality of layer and/or the existence of interface plays a role for the increase in ANE. This means that metallic multilayers or superlattices with a number of interfaces are promising for achieving large ANE.

In this talk, we introduce our recent studies on the ANE using the Ni / Pt metallic superlattices [1] and the Co_2MnGa / AlN multilayers [2]. For the former, the perpendicularly magnetized Ni/Pt (001) epitaxial superlattices were fabricated directly on a non-conductive SrTiO_3 substrate [3], and the Ni layer thickness dependence of ANE was investigated for $[\text{Ni} (t \text{ nm}) / \text{Pt} (1.0 \text{ nm})]_{\times N}$. We found that the values of S^{ANE} for the Ni/Pt superlattices are one order of magnitude larger than that for the bulk Ni. The enhanced ANE is attributable to the large transverse thermoelectric conductivity.

For the latter, the polycrystalline Co_2MnGa / AlN multilayer films were deposited on an amorphous substrate, which shows $S^{\text{ANE}} = 4.9 \mu\text{V K}^{-1}$. This large S^{ANE} is comparable to the values reported for the single crystal Co_2MnGa bulks. The detailed structural analysis and the transport measurement suggest that the effect of interfacial strain on the Seebeck coefficient plays an important role for enhancing the ANE. Since the AlN layer is available on any substrate materials, even on a flexible polyimide substrate, large ANE is successfully achieved for the Co_2MnGa / AlN stack.

Keywords: Metallic Superlattice, Anomalous Nernst Effect, Ordered Alloy, Flexible Substrate

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SD-I06 (Invited)

Extended X-ray Absorption Spectroscopy and Debye–Waller factor under pressure

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The pressure effects on extended X-ray absorption spectroscopy (EXAFS) and the atomic mean-square relative displacement characterizing the Debye–Waller factor have been investigated based on the Debye model [1]. The analytical expressions of the Debye frequency and EXAFS Debye–Waller factor have been derived as functions of crystal volume compressibility. Based on the well-established equation-of-state including the contributions of the anharmonic and electronic thermal pressures [2], numerical calculations have been performed for iron up to a pressure of 220 GPa and compared with experimental data when possible. These results show that the Debye frequency increases rapidly with compression, and beyond 150 GPa it behaves as a linear function of pressure [3]. Meanwhile the mean-square relative displacement curve drops robustly with pressure, especially at pressures smaller than 100GPa. This phenomenon causes the enhancement of EXAFS signals at high pressure. Reversely, the increasing of temperature will reduce the amplitude of EXAFS spectra.

Keywords: High pressure, Melting curves, Vanadium, Niobium, Statistical momentmethod

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SD-I07 (Invited)

Material Properties and Growth Mechanism of β -Ga₂O₃ Epilayers Grown on Sapphire by Metal Organic Chemical Vapor Deposition

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In this study, the monoclinic gallium oxide (β -Ga₂O₃) epilayer was successfully grown on c-plane (0001) sapphire substrate by metalorganic chemical vapor deposition (MOCVD) at different process parameters (growth time, TEGa flow rate and temperature). The surface properties of β -Ga₂O₃ thin film were observed using scanning electron microscopy, atomic force microscope, and X-ray diffraction. The experimental results found that the β -Ga₂O₃ epilayer possess superior crystalline quality that includes (-201), (-402), and (-603) three main crystalline orientations. In addition, by varying the growth time and TEGa flow rate increases, the crystallization characteristics and full width at half maximum of β -Ga₂O₃ film can be effectively improved. The thickness and surface roughness of β -Ga₂O₃ film increase with growth time and TEGa flow rate. However, as the growth temperature increases above 825°C, the thickness of β -Ga₂O₃ film decrease clearly. Furthermore, it can be found that the growth rate decreased as the growth time increasing. Due to the lattice mismatch between the β -Ga₂O₃ and sapphire, the growth mechanism of 3D growth at first, then lateral growth and 2D growth after the thick epilayer being grown was proposed. Furthermore, the β -Ga₂O₃ films are insulating and exhibit high resistance, with a value range of 10^{12} ~ 10^{13} Ω approximately.

Keywords: gallium oxide, metal organic chemical vapor deposition, crystalline, roughness, growth mechanism

SD-I08 (Invited)

Fabrication of Quantum Devices by Fine Sputtering Using a Focused Ion Beam with Nitrogen Gas Field Ion Source

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In fabrication of various quantum devices, nanometer-order fine patterning is usually required. To this end, electron beam lithography (EBL) is frequently and widely used. In this study, instead of EBL, we focused on a focused ion beam with nitrogen gas field ion source (N₂-GFIS-FIB), which has a capability of direct etching by fine sputtering at 10-nm-level or more less [1]. Using this, we fabricated two different types of quantum devices, such as Josephson junction (JJ) devices based on Nb thin film [2] and quantum point contact (QPC) devices based on InGaAs heterostructures [3].

To fabricate JJ devices, we simply performed single line etching of Nb on a semi-insulating GaAs substrate. Figure 1 shows temperature dependence of DC I - V characteristics of a JJ device with inset of a scanning electron microscope (SEM) image. By single line etching of 20-nm-width, a typical JJ behavior can be confirmed.

To fabricate QPC devices, we formed QPC by the direct etching followed by insulator gate stack using atomic layer deposition of Al₂O₃, and evaporation and lift-off of Ti/Au. Figure 2 shows Conductance characteristics of a QPC device with inset of a SEM image. Even though the QPC was depleted at 0 V of gate voltage, conductance was increased and seemed step-like structure with applying positive gate voltage.

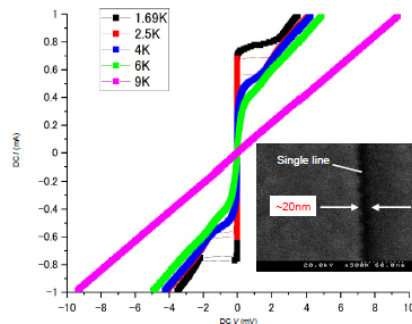


FIG. 1. I - V and SEM image of a JJ device.

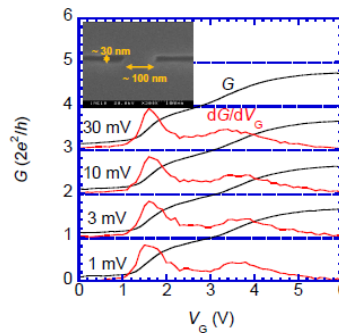


FIG. 2. G - V and SEM image of a QPC device.

Keywords: Gas Field Ion Source (GFIS), Josephson Junction (JJ), Quantum PointContact (QPC)

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SD-I09 (Invited)**Study of nano-scale heat transports using magneto-thermoelectric effects**

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Recent development of nano-fabrication techniques enables to realize functional electronic devices with the lateral dimension down to nano-meter scale. In the operation of such nano sized devices, understanding and controlling the heat transfer is an important issue because a small cross section produces a significant Joule heating effect. Since the characteristic lengths such as the mean free path and phase coherent length are comparable to the device dimension, the heat transport in nanostructured systems may be different from the bulk state and its combination. On the other hand, In the field of spintronics, in addition to the intriguing spin-dependent transports, various conversion phenomena between spin and heat have been reported recently, and a new research field has been emerged named as spincaloritronics. Therefore, it is essential to deepen understanding the heat transfer in nanospintronic devices for manipulating the heat as well as for developing spincaloritronics. In this presentation, we introduce heat-transport phenomena in various ferromagnetic/nonmagnetic metal hybrid structures by using unique magneto-thermoelectric effects.

First, the spatial temperature distribution in a laterally configured nanostructure based on GMR nanowire has been investigated.[1] A large thermal spin valve effect enables us to distinguish the flowing direction of the heat in the GMR nanowire. We find that the heat flow from the substrate is significant. Second, a temperature distribution in a ferromagnetic nanowire has been investigate by using various magneto-thermoelectric effects.[2] The combination between the anisotropic magento- Seebeck effect and anomalous Nernst effect enables us to understand a three-dimension temperature gradient in a ferromagnetic nanowire precisely. We find that the transverse heat flow is a significant contribution on the field dependence of the Seebeck voltage. Finally, temperature dependence of the thermal spin valve effect and anisotropic magneto-Seebeck effect have been investigated. We find that the signs of the voltage changes were reversed at specific temperatures. Possible mechanism has been discussed in order to explain the unique signatures.

Thus, by the optimization of the device structures, enhanced thermal spin valve version of the GMR effect, anisotropic magneto-Seebeck effect and anomalous Nernst effect have been obtained. Multiple ways in which heat interacts with spin and the interplay of such effects enables us to evaluate the heat distribution. These demonstration paves the way for the precise analysis of the heat flow in nano-structured electronic devices.

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SD-I10 (Invited)**Sub-second and ppm-level Optical Sensing of Hydrogen Using Templated Control of Nano-hydride Geometry and Magnetic Composition**Tho Duc Nguyen^{1,*}¹ Department of Physics and Astronomy, University of Georgia, Athens, Georgia 30602, USA

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The use of hydrogen (H₂) fuel as a clean and renewable alternative is one of the most practical solutions for the already serious fossil-fuel shortages, global climate change, and air pollution. However, significant challenges remain with respect to the safe deployment of H₂ fuel sources due to its relatively low ignition energy in a broad flammability range, which is a serious barrier preventing its widespread adoption. Unfortunately, a suite of flammability mitigating technologies, particularly robust sensors for H₂ leak detection and concentration monitoring has not been achieved. To this end, we have developed a class of lightweight optical H₂ sensors based on a metasurface of Pd nano-patchy particle arrays¹, which fulfills the increasing requirements of a safe H₂ fuel sensing system with no risk of sparking. The structure of the optical sensor is readily nano-engineered to yield extraordinarily rapid response to H₂ gas (<3 s at 1 mbar H₂) with a high degree of accuracy (<5%). By incorporating 20% Ag, Au or Co, the sensing performances of the Pd-alloy sensor are significantly enhanced, especially for the magnetic hydride Pd₈₀Co₂₀ sensor whose optical response time at 1 mbar of H₂ is just ~0.85 s, while preserving the excellent accuracy (<2.5%), limit of detection (2.5 ppm), and robustness against aging, temperature, and interfering gases. The superior performance of our sensor places it among the fastest and most sensitive optical H₂ sensors.

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SD-I11 (Invited)

Detection of Weak, Low-Frequency Magnetic Field Using SingleNanoscale MgO Magnetic Tunnel Junctions

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Magnetic tunnel junctions (MTJ) have been widely studied as ultra-sensitive magnetic sensors, due to their high TMR, high sensitivity, excellent scalability and low power consumption [1-3]. In this study, the magnetotransports and noise properties of the 300 nm diameter MTJ at room temperature were investigated. Their sensitivity of more than 100 % in a few Oe at RT. The hard axis bias magnetic field and bias voltage dependence of noise properties both showed that MTJs exhibit relatively low noise spectral density of about which depend inversely on frequency (f) at low frequencies. The noise-based measurement of the developed MTJs is able to detect the present of a nanotesla AC magnetic field ($H_{AC}=6.7$ nT) in the wide range of frequency ($f=100$ -20000 Hz). A noise measurement provides an approach to detect nanotesla-level, low-frequency alternating magnetic fields with a large signal response and contrast-to-noise, presenting an important step in sensing biological fields.

Keywords: Magnetoresistive sensor; tunnel magnetoresistance sensor; magnetic tunnel junctions (MTJ); 1/f magnetic noise

Acknowledgments

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SD-I12 (Invited)**Neutron diffraction study of state-of-the-art 2D materials**Toan Dang^{1,2,*}¹Institute of Research and Development, Duy Tan University, 550000 Da Nang, Vietnam²Faculty of Natural Sciences, Duy Tan University, 550000 Da Nang, Vietnam

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The 2D van der Waals materials with honeycomb magnetic lattice exhibit a large variety of novel physical phenomena due to the interplay of long-range magnetic order and spin fluctuations and they have great potential for technological applications as graphene-like magnetic systems. Recent studies of the model 2D van der Waals compound FePS₃ have revealed structural phase transitions, spin crossover, and emerging superconductivity under high pressure. However, the high-pressure response of magnetic properties of this system remains poorly explored. Here, using the neutron diffraction method, we have observed the emergence of novel magnetic states in FePS₃ under high pressure accompanied by structural transitions. The spin configurations and the formation mechanisms of these phases have been revealed.

Keywords: neutron diffraction, high-pressure, 2D materials, phase transition

Session: Theory and computation
TC-I01 - TC-I10

TC-I01 (Invited)**Thermodynamic properties of the Shastry-Sutherland model for $\text{SrCu}_2(\text{BO}_3)_2$**

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Reliable computation of the low-temperature thermodynamic properties of highly frustrated quantum magnets is important for experiments, but also a considerable challenge since, e.g., conventional Quantum-Monte-Carlo (QMC) simulations suffer from a severe minus sign problem. $\text{SrCu}_2(\text{BO}_3)_2$ is famous for its rich physical properties and as a realization of the two-dimensional spin-1/2 Shastry-Sutherland model. In this model, an orthogonal arrangement of dimers gives rise both to geometric frustration and an exact dimer ground state. Beyond the dimer phase at small inter-dimer coupling, the ground-state phase diagram contains two further phases: an antiferromagnetic one at large interdimer couplings and an intermediate plaquette phase.

We use this example to illustrate recent progress in numerical methods. A QMC method in the dimer basis reduces the minus sign problem sufficiently to be able to obtain accurate results for the specific heat C and the magnetic susceptibility χ in a large part of the dimer phase [1,2]. However, the low-temperature behavior in the parameter regime relevant to $\text{SrCu}_2(\text{BO}_3)_2$ remains out of reach of the QMC simulations. Consequently, we also resort to other methods, in particular a finite-temperature version of the infinite Projected Entangled Pair States (iPEPS) [3].

Application of pressure to $\text{SrCu}_2(\text{BO}_3)_2$ allows to tune the ratio of the coupling constants across the phase transition between the dimer and plaquette phases [4]. High-precision specific-heat measurements demonstrate that the pressure-temperature phase diagram has a first-order transition line that separates phases with different local magnetic energy densities, and that terminates at an Ising critical point. These results are in agreement with results of the numerical methods and reminiscent of the phase diagram of water.

Keywords: Frustrated magnetism, quantum spins models, Quantum Monte Carlo**References**

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TC-I02 (Invited)

The Activation Energy of Glass Transition

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The Arrhenius analysis is a universal tool for studying transitions of the states of materials, owing to the fact that a large number of the transitions have the thermally activated type. The obtained activation energies are well interpreted by the energy barrier separating the terminal states of a transition. Unfortunately, this standard analysis cannot be applied to the glass transition. The temperature (T) dependence of the viscosity at the glass transition often exhibits non-Arrhenius behavior, whereas the so-called strong glasses obey the Arrhenius law. The class of glasses which do not obey the Arrhenius law is called fragile glass. A simple interpretation is that the energy barrier in fragile glass has T dependence. This interpretation seems likely but yet other interpretations are discussed. In either case, the difficulty is its unusually large value of the activation energy Q_a . The value is of the order of 1 eV (sometimes near 10 eV) even for molecular glasses whose melting temperature is less than room temperature. For molecular glasses, Q_a value is even larger than the cohesive energy, which is almost impossible on the physics ground. The glass researchers have been plagued with this problem for a century.

Recently, this problem has been solved by the author [1]. The energy barrier for atom rearrangements significantly changes in the transition range with width ΔT_g . This change in the energy barrier alters the manner in which the apparent activation energy constitutes the Arrhenius form. Analysis of available experimental data shows that the real value of energy barrier is significantly smaller than the apparent activation energy. The overestimation of the apparent activation energy depends on the ratio $T_g/\Delta T_g$, which is larger for fragile glasses than for strong glasses. Importantly, the linear term in the temperature dependence of the energy barrier does not appear in Arrhenius plots. This explains why the T dependence of viscosity for strong glasses obeys well the Arrhenius law, despite that the T dependence of energy barrier is equally expected for every glass. The mechanism of this overestimation was also supported by the specific-heat jump of the glass transition [2].

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TC-I03 (Invited)

Selective Control of Propagation-Conduction of Two Different Quantum Waves by Lattice Imperfections: Electrons and Phonons

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Demands to materials to meet with demands from our societies for our bright future are kept increasingly severe than ever. While conventional theories for materials properties guide us to improve each of materials properties, materials are now required to simultaneously acquire multiple properties, which often go beyond correlated or trade-off relationships among multiple materials properties. Simultaneously to enhance electronic conduction and to suppress thermal conduction by phonons for thermoelectric energy conversion from waste-heat to electricity is just one of many examples being tackled with today and coming years, from liquid-crystal display, Li-ion battery, to advanced turbines for power stations and jet-engines, to name a few.

While machine learning now enable us to explore a room further to find new materials or compounds having new properties whether efficiently or by brute-force, we need to be reminded that there is another room just in front of us: Lattice Imperfections, including point defects including vacancies or dopants, line defects including dislocations, planar defects including interfaces and grain boundaries, all of which significantly modify materials properties, or in other words, materials properties that we know of are due to the lattice imperfections, except in textbooks.

In this presentation, it will be discussed how dislocations, known to dominate plastic deformation or hardness of materials, would selectively modify electronic and thermal conduction in model materials beyond conventional theories.

Keywords: electronic conduction; thermal conduction; ab initio calculations; molecular dynamics; lattice defects

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TC-I04 (Invited)

Computational Approaches to Study Heavy Element Materials

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Heavy elements (lanthanides and actinides), exhibiting interesting chemical and physical properties, are widely used in technological applications. However, due to the complexity of f electrons, *first principles* -based modeling of heavy element materials is largely impacted by time and length scales that need to be accessed. In this talk, I will briefly summarize our recent contributions in the study of these elements: (i) the development of pseudopotentials and basis sets [1, 2] that allow for large scale *ab initio* molecular dynamics (AIMD) simulations; and (ii) an adaptive-learning algorithm [3] that enables the location of multiple low-energy minima in high-dimensional spaces. I will then present applications of these tools to investigate molecular complexes of lanthanides in gas and condensed phases [4, 5]. Finally, I will discuss the use of AIMD and data science in understanding actinide molten salt systems [6, 7].

Keywords: Heavy element materials, ab initio molecular dynamics, data science

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TC-I05 (Invited)

Artificial-neural-network descriptor and interatomic potential for molecular simulations of lattice defects

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In crystalline materials, lattice defects are inevitably introduced due to thermodynamic stability and material fabrication process, having large impacts on material properties. To accurately predict atomic configurations and physical properties of lattice defects with practical computational cost, artificial-neural-network (ANN) interatomic potentials have been employed extensively. However, if an ANN potential learns various atomic environments of lattice defects at once, error with respect to training data becomes large, which leads to severely limited ability to predict lattice defect properties. Consequently, the construction of general-purpose ANN potentials for lattice defects is not yet achieved. To tackle this issue, this work proposed new ANN descriptors and interatomic potentials and compared their error with that of a conventional ANN potential.

For an ANN descriptor, two separate ANNs were used to describe two- and three-body interactions, as shown in Fig. 1. Their outputs were fed to the input nodes of a next ANN. In this architecture, conventional symmetry functions are replaced with the ANN descriptor. Training these three ANNs, the optimal functions of atomic descriptors and interatomic potentials were obtained without manually choosing analytic functions. To generate training and test datasets, DFT calculations were performed using the projector augmented wave method implemented in the VASP code. Here Si was chosen as a model system.

It is found that the ANN-descriptor potential exhibits sufficiently small errors with respect to training datasets, even when the datasets contain various lattice defects including point defects, surfaces and grain boundaries. The mean absolute error (MAE) is calculated to be 0.97 and 2.2 meV/atom for the present ANN potential and a conventional ANN potential, respectively. Our ANN potential is thus expected to exhibit higher predictive ability to lattice defects properties. The trained three-body ANN descriptor is found to involve complicated functional forms (Fig. 2), which cannot be constructed using a single trigonometric function. This may be a reason that our ANN potential shows the lower MAE than that of a conventional ANN potential.

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Keywords: Interatomic potential, Machine learning, First-principles calculation

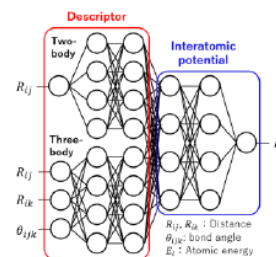


FIG. 1. ANN descriptor and interatomic potential.

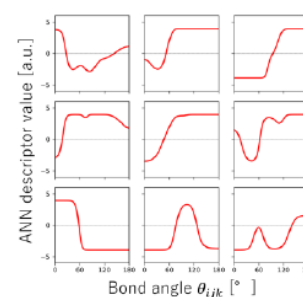


FIG. 2. Trained three-body ANN descriptors

TC-I06 (Invited)

Accelerating Materials Discovery using Universal Neural Network Potential and Ab-initio Calculations

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The discovery of novel materials with good performance for specific applications has been a hot topic in the field of materials science. In this talk, two cases of materials discovery approaches and results in the fields of Li-ion batteries and terahertz (THz) devices will be presented. In the first case, traditionally, materials discovery often consumes a vast amount of time and resources in experiments and computational simulation due to the limitations of experimental conditions or theoretical foundations. Thus, it is crucial to approach this task in a new way. One is the use of neural network potentials, which model the interactions of atoms by mimicking the neural networks in the human brain. In this work, by using the recently developed universal neural network potential, PFP (Preferred Potential) [1], simulations of the delithiation process in Li-ion battery cathode materials will be demonstrated. Also, in combination with Wang-Landau sampling [2], a screening scheme for exploring cathode materials will be introduced. In this scheme, the total energy is calculated quickly and accurately using the PFP, while the thermodynamic properties of the searched compound are determined by using Wang-Landau sampling. For the second case, first-principles methods based on spin density functional theory and *ab-initio* multichannel Landauer formalism for spin-transport will be introduced. These were applied to calculate the spin-dependent interface resistance in the Fe/Pt bilayer used as a spintronic THz emitter [3, 4]. In this research, we found that spin-up interface resistance is lower than that of spin-down, in agreement with previous interface reflectivity studies. The above-mentioned theoretical methods can also be used to predict interface resistances, which are more directly and experimentally measurable than reflectivity and thus spin-injection efficiency of other candidate metal bilayer systems for the accelerated search for efficient spintronic THz emitters.

Keywords: Li-ion Battery, Terahertz Device, Neural Network Potential, Wang-Landau Sampling, Ab-initio Calculation

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TC-I07 (Invited)

Exploration for non-perovskite proton-conducting oxides using high-throughput computation and machine learningS. Fujii^{1,2*}, Y. Shimizu^{3,4,5}, J. Hyodo^{3,5}, A. Kuwabara², Y. Yamazaki^{3,4,5}¹ Division of Materials and Manufacturing Science, Osaka University, Osaka 565-0871, Japan² Nanostructures Research Laboratory, Japan Fine Ceramics Center, Nagoya 456-8587, Japan³ INAMORI Frontier Research Center, Kyushu University, Fukuoka 819-0395, Japan⁴ Department of Materials, Kyushu University, Fukuoka, 819-0395, Japan⁵ Kyushu University Platform of Inter-/Transdisciplinary Energy Research (Q-PIT), Kyushu University, Fukuoka, 819-0395, Japan

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Proton-conducting oxides have attracted attention as electrolytes for solid oxide fuel cells (SOFCs). Perovskite has been considered as the most promising candidates for the electrolytes, and highly conductive Sc-doped BaZrO₃, for example, have been developed recently [1]. On the other hand, there are limited reports on proton-conducting oxides with non-perovskite structures [2]. This is due to the complex nature of proton-conducting oxides, which requires a suitable acceptor dopant to create oxygen vacancies, ease of hydration, crystal structure where protons easily migrate, chemical stability, and so on. It is challenging to find one that meets these requirements simultaneously among the vast number of host compound and dopant combinations.

Here, we developed a scheme of high-throughput *ab initio* computational screening for exploring proton-conducting oxides [3]. This scheme includes multiple stages of bandgap, hydration, proton migration pathways, thermodynamic stability, and solubility of dopants. The screening results show that, although there are many compounds that hydrate once oxide-ion vacancies are formed, very few of them form proton conduction pathways and have dopants that are easily soluble. Based on this computational screening, we successfully synthesized a new proton-conducting non-perovskite oxide for the first trial in experimental synthesis.

Big data obtained by this screening, which includes both non-perovskite and perovskite oxides, is essential for general understanding of the inherent nature of proton-conducting oxides. For this perspective, prediction models for hydration energies and solution energies of dopants were also developed using machine learning. The interpretation of these models clearly highlights the physicochemical properties necessary for proton conduction. In this presentation, the details of the computational methodology, the characteristics of the discovered compounds, the approach of machine learning, and the understanding gained will be discussed.

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Keywords: proton-conducting oxides; high-throughput calculations; machine learning

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TC-I08 (Invited)

Computational materials design of high-entropy alloys based on FPKKR-CPA calculations and machine learning techniques

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High-entropy alloys (HEAs) are composed of more than 5 different elements with nearly equal atomic concentration, and are attractive materials due to their possibility to realize various functionality depending on the choice of the kinds of elements. However, a number of combinations is too large, so exhaustive materials search by experiments is impractical. Recently, first-principles calculations are combined with machine learning techniques to obtain prediction models for physical properties of interest and applied to design new HEAs [1]. In this paper, as one of such attempts, we demonstrate that the combination of the full potential Korringa-Kohn-Rostoker coherent potential approximation (FPKKR-CPA) [2] and the linearly independent descriptor generation (LIDG) method [3] works reasonably and effectively for the prediction of elastic and magnetic properties of HEAs.

Firstly, we try to construct a prediction model of elastic constants of HEAs. Total energy calculations are performed within the framework of the DFT by systematically applying deformations. By using the FPKKR-CPA method one can calculate configuration average of the electronic structure of disordered HEAs without using a large super-cell. The elastic constants are calculated for randomly sampled BCC equi-atomic quinary HEAs composed from 25 transition metals. Then linear regression is performed on calculated elastic constants. The descriptors of the regression are generated by the LIDG method from arithmetic means and standard deviations of 3 independent elastic constants, lattice constant, group and period of elements, atomic number and electron density parameter r_s of components of HEA. By optimizing the combination of descriptors by the genetic algorithm, we can achieve comparable accuracy to the model generated by the neural network. Based on the model, we discuss chemical trend of elastic constants. Similar procedure can be utilized to construct a linear model for predicting magnetic properties of HEAs.

Next, we assess the stability of HEAs. For this purpose, we calculate not only the heat of formation of HEAs but also effective pair interactions (EPIs) between constituent atoms by the generalized perturbation method [4]. We perform Monte Carlo simulations with using the calculated EPIs and simulate temperature dependence of the short-range order in HEAs. This method might help to pick up a candidate HEA from a view point of synthesizability.

Keywords: first-principles calculations, machine learning, high entropy alloy

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TC-I09 (Invited)

Accelerating materials science with artificial intelligence

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Computational materials science has been driven by traditional physics-based approaches, in which physics and chemistry concepts are employed to understand materials (generally solids) from their atomic-scale information. Challenges of such approaches, which range from the technical side, e.g., enormous computational facility and time are required for a meaningful simulation, to a more fundamental level, e.g., how to describe a material and its properties by a model, are never trivial. During the last decade, artificial intelligence (AI) is joining the mainstream of materials research, creating a subfield named materials informatics. In this research area, AI-based approaches are used to complement and significantly accelerate the traditional computational and experimental approaches in understanding, optimizing, discovering, and designing new functional materials, especially those with targeted properties. In this talk, I will outline the fundamental and technical aspects of the AI-based approaches and illustrate them by some of my works in materials informatics. Then, I will offer my outlook on remaining challenges that need to be surmounted for widespread adoption of AI-based approaches in materials science and engineering.

Keywords: Materials science, Materials informatics, Materials discovery & design, Artificial intelligence, Machine learning

TC-I10 (Invited)

Material Intelligence: In-Materio Reservoir Computing Devices Composed by Random Network of Nanoparticles

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The superior computational capabilities of software-based deep learning have been widely recognized, and the practical application of artificial intelligence is rapidly expanding. Meanwhile, attempts to replace artificial intelligence (AI) algorithms with hardware have also begun. We have shown that the properties of materials can be treated as physical phenomena and are conducting research to realize a new form of AI hardware. I will share our recent outputs at the presentation.

In recent years, there is a growing interest in hardware technologies that physically implement artificial neural networks (ANNs), neuromorphic or brainmorphic information processing systems, and the applications (AI systems hereafter), as well as new materials and devices. A critical difference between the presently required device functionality and that in conventional computational systems is the use of chemical dynamics. By cleverly using nanomaterials' nonlinearity and network structure, devices that spontaneously generate pulses, noise, and other physical phenomena are expected to be realized to utilize for the AI hardware. These devices will enable drastically lower power consumption and higher integration of AI systems. In the learning process of ANNs, it is necessary to constantly change and store the weights of the weighted sum (sum-of-products) part. We have been working on materials that can complement CMOS for AI systems by using molecules and nanocarbon materials, and further, we are trying to apply them to autonomous AI robots. This paper introduces these nanomaterials and networks' formation as AI devices [1], the key points of the devices' functionalization, application to robots, and other recent research results [2]-[7].

Keywords: Neuromorphic Hardware, Physical Reservoir Computing, Random Network, Chemical Dynamics, Robot Operating System

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