The Golden Academy Conference Series

2021 Global Research Efforts on Energy and Nanomaterials (GREEN 2021)

Dec 17 - Dec 19 2021

Conference Proceedings

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ASIA PACIFIC SOCIETY FOR MATERIALS RESEARCH

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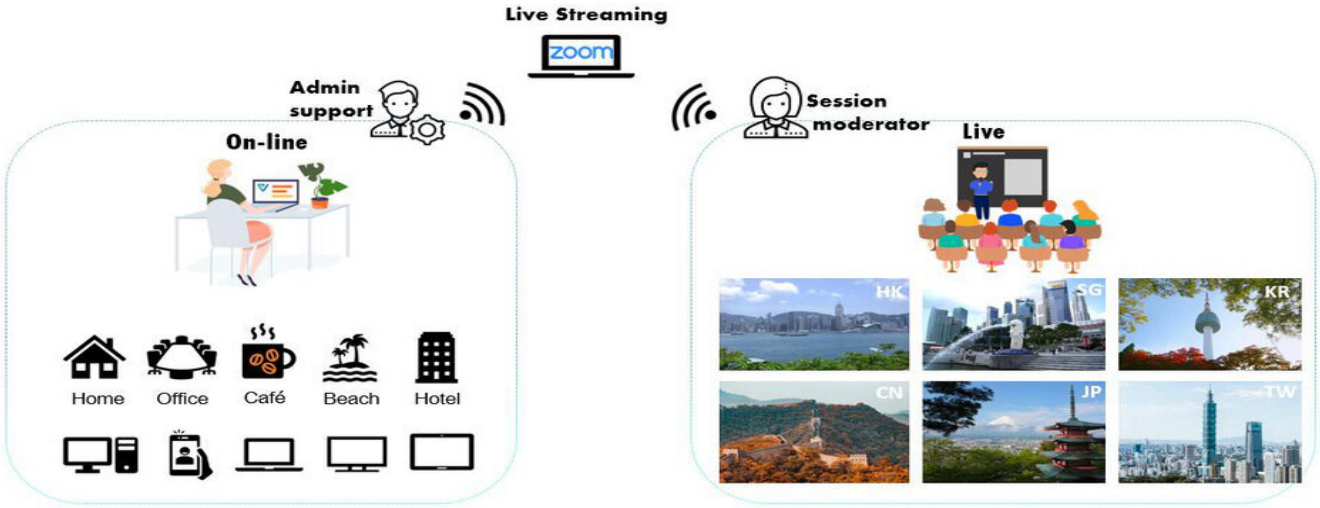
Message from the organizers

Dear Colleagues and Friends,

We would like to invite all of you to join the 2021 Global Research Efforts on Energy and Nanomaterials (GREEN 2021), which will be held during Dec 17-19 2021.



The conference is intended to serve as an interdisciplinary platform for the exchange and networking between top scientists, experienced engineers, frontier researchers, and students across a wide spectrum of research fields.

Your active participation and discussion is the key to the success of this conference.

Yours Sincerely,

GREEN 2021 Committee
Asia Pacific Society for Materials Science (APSMR)
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Conference topics

1. Structure materials and Functional Coatings (metals, ceramics, and composites)
2. Materials for energy (saving, conversion, transfer, storage) and environment plus electrochemistry
2.1. Photovoltaics
2.2. Batteries and Fuel Cells
2.3. Materials for Thermal Management and Thermal Energy Utilization
2.4. Materials for Energy and Environmental Applications
3. Optics and Photonic Materials
4. Electronic, Magnetic and Nanomaterials
5. Polymer Science and Molecular Chemistry
6. Organic Materials and Bio-materials
7. Materials Characterization and Computational Modeling

Beijing/Taipei/Singapore/ Hong Kong	Tokyo/Seoul	FRI, 12/17	SAT, 12/18	SUN, 12/19
9:00-10:10	10:00-11:10	Oral Presentation		
10:10-10:20	11:10-11:20	Break		
10:20-11:30	11:20-12:30	Oral Presentation		

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Presentation List

Beijing/Taipei/Singapore/ Hong Kong	Tokyo/Seoul	FRI, 12/17	SAT, 12/18	SUN, 12/19
9:00-10:10	10:00-11:10	1. A.K. JHA 2. S. CHO 3. K.I. LEE	7. S. YOSHIMURA 8. S. RATHA 9. Y.G. SO	13. Y. ZHANG 14. J.A. JACKMAN 15. R.T. WU
10:10-10:20	11:10-11:20	Break		
10:20-11:30	11:20-12:30	4. J.Y. WU 5. F.B. WU 6. Reserved	10. C.L. HO 11. S. NARITA 12. R.T. WU	16. M. HARUTA 17. S.J. CHENG 18. Z.H.XIE & K.B. ZHENG

GOLDEN ACADEMY

FRIDAY 12/17

1. Evolution of REBCO thin films and their role in promoting sustainable energy (A.K. JHA)
2. Thickness-Controlled Black Phosphorus Tunnel Field-Effect Transistor for Low Power Switches (S. CHO)
3. On the Mechanisms and Mitigation of Volcanic Ash Attack on YSZ Thermal Barrier Coatings (K.I. LEE)
4. Fabrication and application of highly stable PCM nano-emulsions for cooling energy storage (J.Y. WU)
5. Manufacture, Microstructure, and Mechanical Properties of Sputtering Transition Metal Nitride Protective Layers (F.B. WU)
6. Reserved

SATURDAY 12/18

7. Development of high quality BiFeO3-based multiferroic thin films with excellent magnetic properties for realization of high performance and low power consumption magnetic devices (S. YOSHIMURA)
8. Effect of Lanthanoid (L = La, Nd, Sm, Gd, Dy) substitution on various magnetic properties of (Bi,L)(Fe,Co)O3 ferromagnetic and ferroelectric thin films (S. RATHA)

9. Facile synthesis of B20-type FeGe alloys via dilute Si-doping and mechanical alloying (Y.G. SO)
10. New Functional Materials for Photocatalytic Hydrogen Production from Water (C.L. HO)
11. Substitution effect on magnetic properties of β-Mn-type Co–Zn-based alloys (S. NARITA)
12. TGO residual stress characterization using PLPS (R. WU)

SUNDAY 12/19

13. Enhanced dynamic mechanical properties and resistance to the formation of adiabatic shear band by Cu-rich nano-precipitates in high-strength steels (Y. ZHANG)
14. Supported Lipid Bilayer Platform for Studying Multivalent Ligand-Receptor Interactions: A Nanoplasmonic Sensing Study (J.A. JACKMAN)
15. On the interfacial stability of thermal barrier coatings (R.T. WU)
16. Small imaging device for observing dynamics of the plant leaves (M. HARUTA)
17. Revealing Optical Signatures of Momentum Forbidden Dark Excitons in Transition Metal Dichalcogenide Monolayers (S.J. CHENG)
18. TBA (Z.H. XIE & K.B. ZHENG)

Conference Presentation Abstracts

GOLDEN ACADEMY

Fri/12/17

Abstract ID: 1

Evolution of REBCO thin films and their role in promoting sustainable energy

Alok K. JHA, Kyushu Institute of Technology, Japan

The discovery of superconductivity in cuprate oxides in late eighties raised hopes for using these materials in efficient and advanced technological applications. Superconductivity was observed in YBa2Cu3O7-□ (YBCO) and other REBCO (RE = Sm, Gd, Eu etc.) materials in their bulk polycrystalline form. However, the critical current density (Jc) values of the polycrystalline samples were too low to be considered useful for applications. Within a couple of years, it became possible to synthesize highly oriented thin films of YBCO and REBCO superconductors on single crystal substrates. Further, the development of biaxially textured metallic tapes as substrates for REBCO thin films raised the hopes of using them in transmission cables and high-field magnets. Although the reduction of Jc in applied magnetic fields remained a challenge for long time. Further, the development of artificial pinning center (APC) technology has resolved this issue to a large extent. The widespread technological application of REBCO superconducting thin films principally depend on their high critical current density (Jc) and irreversibility field (Hirr) at 77 K. However, it is strongly desired to improve their Jc over wide range of temperature and applied magnetic field [1].

In this talk, the developments in improving the superconducting parameters of REBCO over the years will be presented. In addition, the reduction and control of critical current anisotropy of REBCO thin films through APC technology will also be addressed.

References

1) A. K. Jha and K. Matsumoto, Front. Phys. 7, 82 (2019).

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Fri/12/17

Abstract ID: 2

Thickness-Controlled Black Phosphorus Tunnel Field-Effect Transistor for Low Power Switches

Sungjae CHO, Korea Advanced Institute of Science and Technology, Korea

The continuous transistor down-scaling has been the key to the successful development of the current information technology. However, with Moore's law reaching its limits the development of alternative transistor architectures is urgently needed. Transistors require at least 60 mV switching voltage for each 10-fold current increase, i.e. subthreshold swing (SS) 60 mV/dec. Alternative tunnel field-effect transistors (TFETs) are widely studied to achieve a sub-thermionic SS and high I60 (current where SS becomes 60 mV/dec). Heterojunction (HJ) TFETs bear promise to deliver high I60, but experimental results do not meet theoretical expectations due to interface problems in the HJs constructed from different materials. Here, we report a natural HJ-TFET with spatially varying layer thickness in black phosphorus (BP) without interface problems. We achieved record-low average SS over 4 decades of current, SSave_4dec ≈ 22.9 mV/dec with record-high I60 (= 19.5 μA/μm), paving the way for the application in low power switches.

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Fri/12/17

Abstract ID: 3

On the Mechanisms and Mitigation of Volcanic Ash Attack on YSZ Thermal Barrier Coatings

Kuan-I LEE, The University of Manchester, UK

Yttria stabilized zirconia (YSZ) made thermal barrier coatings (TBCs) have been widely applied to aero engines for decades. When engines are in operation, airborne particles, dusts and ashes could be injected into engine, which then melt and deposit on turbine blades, forming calcium-magnesium-alumino-silicate (CMAS). This substance penetrates into TBCs, both chemically and mechanically damaging the integrity of the YSZ top coat. For the state-of-the-art TBC technology, two major techniques have been developed to mitigate the CMAS attack: 1) modifying the YSZ topcoat chemistry by elemental doping, 2) fabricating a protective overlay on top of YSZ. With these two techniques, alumina is the most common material chosen to prevent CMAS attack. In this study, real volcanic ash is utilized to study the degradation process of TBCs and potential mitigation mechanisms.

Results show that similar to CMAS, volcanic ash penetrates severely through the thickness and fills the columnar gaps of TBC top coat. It is also found that yttria content of the YSZ top coat decreases substantially upon high temperature exposure to volcanic ash, which has detrimental implication to the phase stability of YSZ. With respective to mitigation, volcanic ash reacts with alumina around 1310°C, forming anorthite ($CaAl_2Si_2O_8$), magnetite (Fe_3O_4), and spinel ($Al_{1.75}Mg_{0.889}Mn_{0.351}O_4$) as reaction products, which according to the literature, have melting temperatures above that of the volcanic ash studied and typical values reported for CMAS. As the new melting temperatures are now above typical surface operating temperature of turbine components, melting induced penetration of volcanic ash and CMAS can be suppressed considerably

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Fri/12/17

Abstract ID: 4

Fabrication and application of highly stable PCM nano-emulsions for cooling energy storage

Jianyong WU, Liu LIU, Jianlei NIU, The Hong Kong Polytechnic University, Hong Kong

Phase change materials (PCMs) are useful media for latent energy storage in thermal energy storage (TES) systems. Our group is specially interested in the development and application of PCM emulsions in fluid TES systems. However, PCM emulsions are thermodynamically unstable owning to their high surface free energy. Reduction of the droplet size to the nanoscale or the formation of PCM nano-emulsions is one of the most effective approaches for improving the emulsion stability. In our recent study, highly stable nano-emulsions of n-hexadecane as the PCM component dispersed in water were prepared by the phase inversion temperature (PIT) method. The stability was further improved by the use of two-surfactant combinations, i.e. Brij L4 as the primary surfactant and Tween 60, Tween 80 or polyethylene-block-poly(ethylene glycol) as a co-surfactant. The optimized PCM nano-emulsions showed an excellent stability over 120 days and 300 thermal cycles with a droplet size below 80 nm as well as the desirable Newtonian fluid behaviour with a relatively low viscosity of 50 mPa·s. The nano-emulsion has been successfully tested in a pilot tubular exchanger TES system for building air-conditioning (cooling) application in the working temperature range of 10-15oC, and the related findings will be presented on the conference.

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Fri/12/17

Abstract ID: 5

Manufacture, Microstructure, and Mechanical Properties of Sputtering Transition Metal Nitride Protective Layers

Fan-Bean WU, Kun-Yuan LIU, Ya-Yuei YANG, Jan-Yin XIANG, Zen-Xin LIN, Yu-Chen LIU, National United University, Taiwan

Transition metal nitride, TMN, layers have been applied for the enhancement in surface protection applications due to their advantages in high hardness, elastic modulus, adhesion, wear and corrosion resistance. The TMN films can be fabricated in single-, dual-, multi-element, and multilayer nitride systems, which attracted intense attentions due to theirs structure features and specific strengthening mechanisms. In this work, single-layer TaN and MoN single transition metal nitride layers and multilayer coatings, dual-element (MoHf)N nitride layers, are deposited through vacuum sputtering process. Film configuration is identified since distinct crystal structures, like columnar crystalline, nanocrystalline, and even amorphous features, are manipulated for building layers. The mechanism of film growth is discussed through deposition parameters, including gas mixture, sputtering power density, sequential, and co-sputtering deposition methods. The distinguishable interfaces in the multilayers could be established by different microstructure of adjacent layers. The higher power and larger N2 gas inlet during deposition generated amorphous layers and suppressed the growth of continuous columnar crystals in layers. The multiple-phase and solid-solutioning are the strengthening mechanisms for dual-element TMN coatings. The hardness, elastic modulus, indentation cracking behavior, tribological characteristics are evaluated and taken as indicators of protective properties for versatile TMN films.

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Fri/12/17

Abstract ID: 6

TBA

Reserved

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Sat/12/18

Abstract ID: 7

Development of high quality BiFeO3-based multiferroic thin films with excellent magnetic properties for realization of high performance and low power consumption magnetic devices

Satoru YOSHIMURA, Akita University, Japan

Magnetic reversal method using an electric field is a future technology for high performance magnetic devices with lower power consumption. Multiferroic (ferromagnetic and ferroelectricity) materials with magneto-electric effect have been receiving greater attention for this method. Ba or La doped BiFeO3 (BiFeO3 is typical material with antiferromagnetic and ferroelectricity) were reported as multiferrioc material with clear ferromagnetic hysteresis. Although the excellent magnetic properties such as high saturation magnetization, perpendicular magnetic anisotropy, and large magnetic Kerr effect are needed to realize the high performance magnetic devices, the magnetic properties of Ba or La doped BiFeO3 thin films are not sufficient for application to that magnetic devices. To realize those magnetic properties, substitution of Co against Fe in (Bi1-xBax)FeO3 and (Bi1-xLax)FeO3 were investigated in this study. In the (Bi,Ba)(Fe,Co)O3 thin films, Co substitution of 20 % had contribution to increase the saturation magnetization, magnetic anisotropy, and magnetic Kerr effect. The highest saturation magnetization of around 100 emu/cm3 was obtained in (Bi1-xBax)(Fe1-yCoy)O3 thin films with the total composition of Ba and Co of around 60 %. Further increase of Ba and Co substitution decreased the saturation magnetization and perpendicular magnetic anisotropy because the formation of the BiFeO3 phase is hindered by an excess amount of Ba and Co with larger ion radius than Bi and Fe. In the (Bi,La)(Fe,Co)O3 thin films, Co substitution up to 30 % had contribution to increase the saturation magnetization, magnetic anisotropy, and magnetic Kerr effect. Here, in the case of Bi(Fe,Co)O3, it is known that Co substitution increases the saturation magnetization but does not change the magnetic anisotropy. Therefore, it is considered that the mechanism to improve the magnetic properties by Co substitution especially magnetic anisotropy is different depending on the presence or absence of element substitution at the Bi site.

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Sat/12/18

Abstract ID: 8

Effect of Lanthanoid (L = La, Nd, Sm, Gd, Dy) substitution on various magnetic properties of (Bi,L)(Fe,Co)O3 ferromagnetic and ferroelectric thin films

Soumyaranjan RATHA, Kotaro TAKEDA, Munusamy KUPPAN, Genta EGAWA, Satoru YOSHIMURA, Akita University, Japan

(Bi0.5L0.5)(Fe0.75Co0.25)O3 (L=La, Nd, Sm, Gd, Dy) films (200 nm) with ferromagnetism and ferroelectricity properties were fabricated onto Ta (5 nm) / Pt (100 nm) underlayers with various substituting materials L against Bi using a UHV sputtering system to obtain high saturation magnetization (Ms), perpendicular magnetic anisotropy, and large magnetic Kerr effect (Θk) in this study. In multiferroic (ferromagnetic and ferroelectric) material, the magnetization direction is controlled by voltage provided. So, these magnetic properties are very important for realization of high performance magnetic devices driven by electric field. All synthesized (Bi0.5L0.5)(Fe0.75Co0.25)O3 (L=La, Nd, Sm, Gd, Dy) films had relatively high Ms of more than 75 emu/cm3, perpendicular magnetic anisotropy (perpendicular coercivity (Hc⊥) / in plane coercivity (Hc//) of more than 1.3), and Θk of more than 0.2 degree. Especially, (Bi0.5Nd0.5)(Fe0.75Co0.25)O3 film had a very high Ms of 140 emu/cm3, which is suitable for realization of high sensitivity sensor devices and new magnetic devices with magnetization transfer system. (Bi0.5Gd0.5)(Fe0.75Co0.25)O3 film had a high Hc⊥/ Hc// of 2.7, which is suitable for realization of large capacity magnetic memory devices, (Bi0.5La0.5)(Fe0.75Co0.25)O3 film had a very high Θk of 0.72 degree, which is suitable for realization of high resolution magnetic-optical devices, and (Bi0.5Dy0.5)(Fe0.75Co0.25)O3 had a high Hc⊥ of 5.0 kOe, which is suitable for realization of high density recording media of hard disk drive. These magnetic properties were excellent compared with the case of typical multiferroic (Bi0.5A0.5)FeO3 (A=Ca, Sr, Ba) films with the maximum value of Ms as 90 emu/cm3, Hc⊥/ Hc// as 0.8, and Θk as 0.03 degree, which were fabricated previously in our group. These magnetic properties of BiFeO3 based material with substitution of Lanthanoids against Bi are very important for realization of high performance magnetic devices driven by electric field.

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Sat/12/18

Abstract ID: 9

Facile synthesis of B20-type FeGe alloys via dilute Si-doping and mechanical alloying

Yeong-Gi SO, Akita University, Japan

Magnetic skyrmions exhibit excellent potential for use in future data storage devices because of their topological stability at nanometer-scale dimensions. FeGe alloy with a B20-type structure is a typical example of chiral magnets that host stable magnetic skyrmions. Although B20-type FeGe alloys that host skyrmions have been intensively studied, their synthesis processes have so far been limited to high-pressure and high-temperature (HPHT) synthesis methods. Herein, we report two facile synthesis methods of B20-type FeGe alloys without employing a HPHT: dilute Si-doping and mechanical alloying. Through conventional alloying combined with Si doping, we achieved the formation of a well-defined B20 phase. We also applied mechanical alloying to synthesize various B20-type transition-metal monogermanides and successfully obtained several binary and ternary B20-type alloys as well as B20-FeGe. In this talk, detailed experimental results, including the formation conditions and magnetic properties of B20 alloys, will be presented.

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Sat/12/18

Abstract ID: 10

New Functional Materials for Photocatalytic Hydrogen Production from Water

Cheuk-Lam HO, The Hong Kong Polytechnic University, Hong Kong

Since the quality of our life depends on a large extent on the availability of energy, the energy crisis problem will pose a great threat to us for the foreseeable future and energy is and will certainly remain one of the great challenges for the world. It is critically essential to find alternative forms of renewable energy sources. The transformation of solar light into chemical fuels, especially hydrogen, through solar-driven photocatalytic reaction is an important area. Development of functional organic molecules as photosensitizers and catalysts to capture solar light have become a field of intense activities in the photocatalytic research. The chemical and physical properties of such functional materials can be easily fine-tuned simply by varying its chemical structures to develop the best materials to fit for solar-to-hydrogen application. This lecture presents a critical perspective of the field, with emphasis on fundamental structural design concepts of molecular photosensitizers and catalysts and their current applications.

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Sat/12/18

Abstract ID: 11

Substitution effect on magnetic properties of β-Mn-type Co–Zn-based alloys

Souki NARITA, Yeong-Gi SO, Akita University, Japan

The rapidly developing information society today demands memory devices with high density and low power consumption. To this end, nanoscale vortical magnetic structures called skyrmions that can serve as magnetic information carriers have been developed. For practical purposes, it is essential to establish a method to control the formation temperature and size of skyrmions. The recently discovered skyrmion host-material, the Co10-x/2Zn10-x/2Mnx alloy with the β-Mn type structure, shows extensive variations in formation temperature and skyrmion size depending on its Mn content. To better understand the substitution effect of dopant elements on the magnetic properties of β-Mn-type alloys, exploration of different β-Mn-type alloys that can host skyrmions is important. Herein, we investigated the formation and magnetic properties of a series of β-Mn-type Co-Zn-M (M= Ga, Al, Fe) alloys. We found that Ga or Al could be substituted with Zn in the new β-Mn-type Co50Zn50-xMx alloys; this substitution had a negligible effect on the Curie temperature (Tc). In contrast, Fe was substituted with Co, and Tc varied with the Fe content. Furthermore, we proposed the mechanism underlying the substitution effect on the magnetic properties.

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Sat/12/18

Abstract ID: 12

TGO residual stress characterization using PLPS

Rudder WU, Ye CHEN, Xiangtan University, China

Photo-stimulated luminescence piezo-spectroscopy (PLPS) is a well established method used in the characterization of TGO stress state. The frequency characteristics of the Raman peak or the fluorescence peak are sensitive to the strain (stress) of the material, with a corresponding relationship (generally linear) between the two. Based on this characteristic Raman spectroscopy has been widely used in the measurement of residual stress and micromechanical study of thermal barrier coatings (TBC) specimens. In this presentation, preliminary results of measurements on a curved surface using a newly developed PLPS system equipped with an advanced optical assisted autofocus function. The fundamental working principles of PLPS and the measured results will be discussed.

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Sun/12/19

Abstract ID: 13

Enhanced dynamic mechanical properties and resistance to the formation of adiabatic shear band by Cu-rich nano-precipitates in high-strength steels

Yang ZHANG, Harbin Engineering University, China

Yang Zhang is currently an associate professor of Harbin Engineering University. He obtained his Ph.D. degree from Shandong University, China. Then he worked as a postdoctoral researcher at the Pennsylvania State University, USA. His research focuses on the mechanical properties and irradiation effect of nanoprecipitate and nanotwin strengthened alloys. He was awarded for the first prize of Science and Technology Award of Heilongjiang Province. In 2019, he was selected as Youth Talents in Science and Technology of China National Nuclear Corporation. He has published more than 30 SCI papers, including Adv. Sci., Int. J. Plasticity and Appl. Phys. Lett., etc. He has accepted more than 20 invention patents.

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Sun/12/19

Abstract ID: 14

Supported Lipid Bilayer Platform for Studying Multivalent Ligand-Receptor Interactions: A Nanoplasmonic Sensing Study

Joshua JACKMAN, Sungkyunkwan University, Korea

There is broad interest in developing biomimetic membrane platforms to study multivalent ligand–receptor interactions that involve biological nanoparticles such as exosomes and membrane-enveloped virus particles. However, most related measurement strategies focus on nanoparticle attachment while it is far less understood how such interactions induce nanoparticle shape deformations that are believed to play important roles in biological processes. In this talk, I will introduce our group's efforts to develop a nanoplasmonic sensing strategy that enables real-time, label-free tracking of biotinylated lipid vesicle binding to a streptavidin-receptor-functionalized supported lipid bilayer (SLB) platform. Depending on the ligand and receptor fractions in the vesicles and SLB, respectively, we observed variations in the extent of vesicle shape deformation and analyzed the contributing physicochemical factors. Based on the experimental results and theoretical analyses, we identified a critical ligand density corresponding to the onset of significant vesicle deformation and considered the relative interplay of the membrane bending energy and the multivalent binding interaction energy that gives rise to this trend. These findings demonstrate the broad applicability of nanoplasmonic sensing strategies to study nanoparticle shape changes related to multivalent ligand–receptor systems.

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Sun/12/19

Abstract ID: 15

On the interfacial stability of thermal barrier coatings

R.T. WU, Xiangtan University, China

Efficient energy use, sometimes simply referred to as energy-saving, involves efforts to reduce the amount of energy wasted. To minimize heat loss and improve energy utilization, materials with ultra-low thermal conductivities are becoming increasingly important under the growing demand for high performance thermal management. Thermal barrier coatings (TBCs) based on yttria stabilized zirconia are widely used in advanced aerospace applications as high temperature thermal insulation materials. In this workshop, I will be presenting my research activities on understanding the interfacial stability and factors controlling thermal, micro-mechanical and physical properties of these materials.

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Sun/12/19

Abstract ID: 16

Small imaging device for observing dynamics of the plant leaves

Makito HARUTA, Minoru KUBO, Hironari TAKEHARA, Nara Institute of Science and Technology; Hiroyuki TASHIRO, Nara Institute of Science and Technology & Kyushu University; Kiyotaka SASAGAWA, Jun OHTA, Nara Institute of Science and Technology, Japan

In recent years, remote sensing technologies based on field servers have been developed for monitoring crop growth status and agricultural production. However, these methods used large-scale devices. It is difficult to observe the state of plant tissue in real-time. For remote sensing for observing the plant tissue in detail, small-size and high-sensitivity devices are required.

In this study, we have developed a small imaging device for observing the dynamics of the plant leaves. This device composed a CMOS image sensor, a fiber optic plate (FOP), and LEDs for illumination. To protect the sensor from scuffs and moisture, the FOP is placed on the sensor's surface. Green LEDs with an emission wavelength of 525 nm are located on the opposite side of the sensor as a light source for observing the surface of the leaf. The light around this wavelength is absorbed little by the chloroplast. This device uses a contact imaging method for getting high spatial resolution and wide range with a simple structure. The Raspberry pi 4B and Python 3 controlled the CMOS image sensor and LEDs for generating time-lapse imaging. Using the miniature real-time monitoring device, we demonstrated successful observation of microscopic-scale structures in plant leaf tissue and their physiological responses. This device, which can acquire high-resolution images, can clearly capture the state of leaf vein cells and stomata. In the future, we aim to achieve long-term measurement and evaluation of physiological activity during plant photosynthesis and the progression of lesions.

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Sun/12/19

Abstract ID: 17

Revealing Optical Signatures of Momentum Forbidden Dark Excitons in Transition Metal Dichalcogenide Monolayers

Shun-Jen CHENG, National Yang Ming Chiao Tung University, Taiwan

Atomically thin transition-metal dichalcogenide monolayers (TMD-MLs) such as MoS2 and WSe2 monolayers have recently received broad attention because of the intriguing spin-, valley-, and excitonic properties. Because of poor screening in low dimensionality, Coulomb interaction in TMD-MLs is dramatically enhanced. Thus, photo-generated excitons in TMD-MLs incident are tightly bound and featured with significantly valley and spin-split excitonic fine structures, consisting of the states of various exciton complexes, including bright exciton (BX), spin-forbidden (SF), and various momentum-forbidden (MF) dark exciton (DXs) as well. In particular, despite of violating the momentum selection rules, the MF-DXs in TMD-MLs are recently realized to be essential in various optical and dynamical phenomena but rarely explored yet so far. In this work, we present a comprehensive theoretical investigation of the full excitonic fine structures of WSe2-MLs by solving the density-functional-theory (DFT)-based Bethe-Salpeter equation (BSE) with the full consideration of both electron-hole direct and exchange Coulomb interactions. Accordingly, we reveal the optical signatures of the optically inactive MF-DX in temperature-dependent photo-luminescence, in excellent agreement with the existing experimental data. Further, under the guidance of symmetry analysis, we show that the MF-DXs with specific finite momenta inherently possess superiorly high degree of valley and optical polarizations and optically accessible by spatially structured laser beam with optical orbital angular momenta. Those findings shed light on the prospect of valley-based photonics with the utilization of those long-lived, optically accessible, and superiorly valley-polarized MF-DXs.

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Sun/12/19

Abstract ID: 18

TBA

Zhihang XIE, Kunbang ZHENG, Xiangtan University, China

TBA

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