The Golden Academy Conference Series

Asia Pacific Society for Materials Research 2022 Annual Meeting (APSMR 2022 Annual Meeting)

Aug 19 - Aug 21 2022

Conference Proceedings

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ASIA PACIFIC SOCIETY FOR MATERIALS RESEARCH

GOLDEN ACADEMY

Message from the organizers

Dear Colleagues and Friends,

We would like to invite all of you to join the APSMR 2022 Annual Meeting which will be held during Aug 19-21 2022.

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,

APSMR 2022 Annual Meeting Committee
Asia Pacific Society for Materials Science (APSMR)
www.apsmr.org

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Conference organizing committee

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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/Singapore /Taipei /Hong Kong	Tokyo/Seoul	FRI, 08/19	SAT, 08/20	SUN, 08/21
9:00-11:30	10:00-12:30	Oral Presentation		
11:30-13:00	12:30-14:00	Lunch Break		
13:00-16:00	14:00-17:00	Oral Presentation		

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Presentation List

Beijing/Singapore /Taipei /Hong Kong	Tokyo/Seoul	FRI, 08/19	SAT, 08/20	SUN, 08/21
9:00-11:30	10:00-12:30	1. W.C. LIN 2. J. SHI 3. K. TAKAHASHI 4. W. ZHANG 5. X. CUI	12. J.O. LIU 13. F. KAWAGOE 14. Y. SATO 15. Y. NAKAJIMA 16. G. XU	17. S. CHEN 18. T. SAITO 19. K. YAMAMOTO 20. D. LEI 21. H. YAO
11:30-13:00	12:30-14:00	Lunch Break		
13:00-16:00	14:00-17:00	6. R. YAMAZAKI 7. T. OTANI 8. I. MD ALRAZI 9. R. AHMED 10. R. ISHIMATSU 11. T.C. WU		

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FRIDAY 08/19

1. In vivo evaluation of optical values of dental glass-ceramics at different sintering temperatures (W.C. LIN)
2. Synthetic studies of polymers from half-esters obtained by practical selective monohydrolysis reaction and their application to hydrophobic and antifouling modification of graphene oxide (J. SHI)
3. Theoretical understanding on CO2 reduction ethanol production on NiMn@g-C3N4 (K. TAKAHASHI)
4. Characterization and numerical modeling for curing of commercial-grade carbon fiber composite prepregs (W. ZHANG)
5. Performance investigation of a hollow fiber membrane-based evaporative cooler (X. CUI)
6. Strength and fracture of metal-resin joint (R. YAMAZAKI)
7. Surface scratching characteristics of single-crystal silicon (T. OTANI)
8. A novel functional inhibitor of mitotic kinesin Eg5 composed of photoswitching molecular device (I. MD ALRAZI)
9. Ras photocontrol by regulatory factor GAP which has been modified with a photochromic molecular device (R. AHMED)
10. Importance of the electronic structure of luminescent molecules in electrogenerated chemiluminescence (R. ISHIMATSU)
11. On the residual stress of thermal barrier coatings (T.C. WU)

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SATURDAY 08/20

12. Novel macrocycles inspired by natural products (J.O. LIU)
13. Comprehensive synthesis of side-chain fluorinated vitamin D3 analogues：Construction of chemical library and exploration of drug candidates (F. KAWAGOE)
14. Design of lipid nanoparticles for delivery of macromolecules (Y. SATO)
15. Precise synthesis of organosilicon compounds for high-performance materials (Y. NAKAJIMA)
16. TBA (G. XU)

SUNDAY 08/21

17. Short-range ordering and its impact on property of high-entropy alloys (S. CHEN)
18. Progress and prospects of Sm-Fe-N magnets (T. SAITO)
19. New development environment based on digital materials and a case study of PM filter (K. YAMAMOTO)
20. TBA (D. LEI)
21. TBA (H. YAO)

Conference Presentation Abstracts

GOLDEN ACADEMY

Fri/08/19

Abstract ID: 1

In vivo evaluation of optical values of dental glass-ceramics at different sintering temperatures

Wei-Chun LIN, Taipei Medical University, Taiwan

Dental clinics and dental hospitals are being impacted by digitalization and are actively developing a fully digitalized medical process. In prosthodontics, dental prostheses play a huge role in restoring oral function, comfort, appearance and health. At present, the application of materials with strength and high aesthetics as dental restorations is still sought in clinical practice. The excellent mechanical properties and biocompatibility of all-ceramic restorations are popular in dentistry. Many manufacturers are still developing new glass ceramics. The ability of glass ceramics to express the optical properties of natural teeth is an important goal of aesthetic restorations. Dental restorations don't just need to be similar in color to natural teeth. The optical properties of ceramic materials are mainly distinguished by different hues combined with translucency. However, the wide variety of colors requires clinical preparation of ceramic materials in a variety of shades and translucencies to meet the needs of each patient. Therefore, it is expected that glass ceramics can change the crystal size and porosity through different heat treatment temperatures and times, and present different transparency effects. The purpose of this study was to analyze the effect of changes in sintering temperature on the optical properties of glass-ceramics. It is expected that this study can provide a useful contribution to clinical dental restoration.

Notes

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Fri/08/19

Abstract ID: 2

Synthetic Studies of Polymers from Half-esters Obtained by Practical Selective Monohydrolysis Reaction and Their Application to Hydrophobic and antifouling modification of graphene oxide

Jianjun SHI, Hainan Normal University, China; Satomi NIWAYAMA, Muroran Institute of Technology, Japan; Zaifeng SHI, Xiaoxue LIN, Hainan Normal University, China

The polynorbornadienes with cyclopentene backbones are expected to exhibit stiffer properties and higher thermal stabilities due to their rigid architecture. A variety of symmetric and nonsymmetric 2,3-bis(alkoxycarbonyl)norbornadiene monomers were prepared from the half-esters obtained by practical selective monohydrolysis reaction. Libraries of polynorbornadienes were synthesized with good yields with Grubbs 2nd generation catalyst by ring-opening metathesis polymerization (ROMP). The following hydrogenation reactions of the obtained polymers were carried out to yield polymers having saturated structures in the main chains for improvement of the thermal stabilities.

Surface-initiated ring-opening metathesis polymerization (SI-ROMP), based on the design of hydrophobic and antifouling monomers, was employed for the synthesis of grafting-modified grapheme oxide (GO). The copolymers were prepared by employing fluorinated norbornenes (NBFn) and polyethylene glycol-substituted norbornenes (Nb-PEG) as monomers in the presence of Grubbs 2nd generation catalyst. The grafted copolymer films improved the dispersibility of GO in organic solvents and the contact angle. The protein resistance of the modified GO has better antiadsorption ability towards large molecular weight proteins.

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Fri/08/19

Abstract ID: 3

Theoretical understanding on CO2 reduction ethanol production on NiMn@g-C3N4

Kaito TAKAHASHI, Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan

The Electrocatalytic CO2 reduction reaction has attracted the attention of researchers, and there is growing interest in understanding the carbon-carbon (C-C) coupling reaction, which helps form C2 products such as ethylene and ethanol. Here, we focus on theoretically analyzing the effect of diatom NiMn doping on graphitic carbon nitride (g-C3N4), which was experimentally synthesized. We performed analysis along the reaction coordinate of the C-C coupling reaction to understand how the electronic structures of NiMn doped on pristine (NiMn@g-C3N4) and N-vacancy graphitic carbon nitride (NiMn@V-g-C3N4) affect the reaction. Our results show that NiMn@V-g-C3N4 produces ethanol at a low limiting potential of -0.55 V and a low kinetic barrier (0.78 eV) for *CO+*CHO→*COCHO. At this step, electron donation from the N-vacancy substrate to the adsorbate is essential. Discussions on why the additional electron will affect the reaction will also be presented.

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Fri/08/19

Abstract ID: 4

Characterization and Numerical Modeling for Curing of Commercial-Grade Carbon Fiber Composite Prepregs

Weizhao ZHANG, Yuncong FENG, Weike ZHENG, Zhibin HAN, The Chinese University of Hong Kong, Hong Kong

Carbon fiber reinforced polymer (CFRP) has been utilized in a wide range of engineering applications due to its superior properties, including high strength-to-weight ratio, excellent anti-erosion performance and good geometric stability. To manufacture CFRP products, curing of resin matrix is an indispensable step. Due to mismatch properties of thermoset resin and carbon fibers, residual stress is usually generated during curing, causing unwanted deformation. Numerical modeling is a promising and effective approach to predict and assist compensation of curing-induced deformation. As carbon fibers remains both chemically and mechanically stable throughout curing, challenge of curing modeling is mainly caused by resin. A numerical modeling method was developed to predict curing behavior of a prepreg-exclusive thermoset resin, YZ-05. Several modeling components for heat transfer, curing kinetics and viscoelastic constitutive law were developed to fulfill thermo-chemical-mechanical coupled simulation. As YZ-05 exhibits severe creep under high curing temperature, a contactless measurement method involving Digital Image Correlation (DIC) and thermography technique was employed to characterize chemical shrinkage and thermal expansion of the resin. In the aspect of viscoelasticity, time-temperature superposition principle (TTSP) with a new automated shifting algorithm was utilized to construct relaxation master curve from piecewise experimental results. Prediction accuracy of the modeling method for resin curing was validated using experiments where bending of resin beams was introduced in curing. Afterwards, a modeling method for curing behavior of unidirectional (UD) CFRP with YZ-05 matrix was further established. A micromechanical algorithm was introduced to derive viscoelasticity of the composite by combining isotropic viscoelasticity of resin with transverse elasticity of carbon fibers in Laplace domain. Curing experiments under various process conditions demonstrate that prediction accuracy of the modeling methods for both resin and composite curing is less than 7%.

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Fri/08/19

Abstract ID: 5

Performance investigation of a hollow fiber membrane-based evaporative cooler

Xin CUI, Xi'an Jiaotong University, China

Evaporative cooling systems have attracted increasing attention for energy-efficient air conditioning applications. A hollow fiber membrane-based evaporative cooler (HFMEC) is proposed in this study. The selected membrane material can selectively allow only water vapor to penetrate, while preventing the passage of bacteria and fungi, thereby avoiding deterioration of indoor air quality. An experimental setup was developed to study the air treatment performance of the HFMEC under various operating conditions. A numerical model was established and validated. The outlet air temperature predicted by the numerical model using free surface model showed a maximum deviation of 5% comparing with the experimental data. The model was further used to conduct a parametric analysis of the HFMEC. Six key parameters, including geometric specifications and operating conditions, were selected as factors for the sensitivity analysis. The cooling capacity and coefficient of performance (COP) were chosen as performance evaluation indexes. The simulation was performed with 27 cases for the orthogonal test. The results revealed that the inlet air relative humidity, inlet air velocity and packing fraction had significant impact on its cooling capacity and COP. By ranking of the influence degree of selected key parameters on the performance evaluation indexes, the present work proposes a practical approach to design and optimize the counter-flow HFMEC.

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Fri/08/19

Abstract ID: 6

Strength And Fracture of Metal-Resin Joint

Ren YAMAZAKI, Masayoshi TATENO, Kogakuin University, Japan

This study provides a relationship between the interface edge shapes and bonding strength, which is leading to improving the practical bonding strength of PPS resin/aluminum joint specimens. Resin materials are relatively easy to process and work with products. On the other hand, since the strength of resin is lower than that of metals, it tends to be applied for a limited range of use as a material for engineering fields. Therefore, it is important to bond metals, which possess excellent mechanical properties, to resins. Bonded dissimilar materials such as resin/metal joint systems have been developed by taking advantage of them. The strength characteristics and reliability of the bonded systems should be clarified in practical experiments to apply them to many engineering fields of various industries. In this study, the tensile bonding strength of a resin/metal joint system consisting of PPS and aluminum with worked-free surfaces was evaluated experimentally. A preliminary investigation was made to clarify the effect of the storage time after manufacturing the joint systems on the strength and fracture patterns. The geometrical interface edges effects were evaluated experimentally under the time condition when the strength characteristics were constant regardless of time after manufacturing. An improvement effect on the strength by modifying the interface edges was considered based on the practical experimental results.

Notes

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Fri/08/19

Abstract ID: 7

Surface Scratching Characteristics of Single-Crystal Silicon

Tsuyoki OTANI, Masayoshi TATENO, Kogakuin University, Japan

This study provides surface scratch characteristics for the main surface (100) of single-crystal silicon. Since single crystal silicon can be applied to the semiconductor processes, it will be expected as a material used for micromachines. When the single crystal silicon behaves brittlely under room temperature, it is important to have a comprehension of the mechanism for both formation and propagation of the cracks on the surfaces from the viewpoint of ensuring the reliability of the micro-structures. In this study, a scratch testing machine was used for this evaluation to clarify the surface cracks formed on the main surface (100) and the cleavage plane (110) in the silicon wafer. This evaluation provided a scratch characteristic curve, which was the correspondence between the scratch resistance and the vertical load when a scratch needle straightly moved along the scratch direction [110] at a constant speed. After this scratch test, the scratch marks and cracks formed on the main surface and cross-sectional planes were observed using a microscope. An effect of mechanical scratch condition on the crack formation was considered based on the practical experimental results.

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Fri/08/19

Abstract ID: 8

A novel functional inhibitor of mitotic kinesin Eg5 composed of photoswitching molecular device

Islam MD ALRAZI, Shinsaku MARUTA, Soka University, Japan.

Kinesin is an ATP-driven motor protein considered a bio nanomachine. Eg5 is a member of the kinesins group and moves on microtubules by hydrolysis of ATP. It is also known as (KIF 11, KNSL1, and kinesin -5). It reveals that it is essential for forming bipolar spindles during the division of eukaryotic cells. It has been reported that Eg5 expression is much higher in cancer cells than in normal cells. Therefore, it has been thought of as a target for cancer therapy.

Interestingly, tiny chemical compounds that block Eg5 result in the production of monopolar spindles, mitotic arrest, and ultimately cell death. Numerous well-known Eg5 inhibitors, including Monastrol, S-Trityl-L-Cysteine (STLC), Ispinesib, and so on, have been developed as anticancer drugs. They all bind to the same pocket of Eg5, which is made up of the alpha 2, 3, and Loop-5 regions, despite their structural differences and lack of conservation make them all unique. We discovered a novel photochromic compound SPSAB, which composed of spiropyran and azobenzene and inhibited Eg5 in multiple steps as a nanodevice. SPSAB demonstrated three isomer formation states: SP-Trans (VIS), MC- Cis (UV), and MC- Trans (in the dark). In the three states of SPSAB, various inhibitory activities for basal, microtubule stimulated Eg5 ATPase, and microtubule gliding assay were observed. The SP-Trans isomer displayed the most potent inhibitory activity among the three states. We also examined a mixed motor motility assay using conventional kinesin and Kinesin Eg5 to see SPSAB inhibits which phase of the motility cycle. The isomers SP-Trans and MC-Cis showed inhibition like STLC. However, MC-Trans showed a similar inhibition that the inhibitor BRD9876 prevented Eg5 from binding to microtubules in the absence of light. The results suggested that SPSAB may stop the Eg5 ATPase cycle while it was in the ADP state.

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Fri/08/19

Abstract ID: 9

Ras photocontrol by regulatory factor GAP which has been modified with a photochromic molecular device

Rajib AHMED, Nobuyuki NISHIBE, Hideyuki WATANABE, Islam MD ALRAZI, Shinsaku MARUTA, Kondo KAZUNORI, Soka University, Japan

The small GTPase Ras is a central regulator of cellular signal transduction processes leading to transcription, cell cycle progression, growth, migration, cytoskeletal changes, apoptosis, cell survival and senescence, and functions as a molecular nanomachine. The switching mechanism is a well-known thing at the molecular level and considered an intracellular signaling bio nanomachine. It is known that Ras is activated in the guanosine 5'-triphosphate (GTP) bound state and inactivated in the GDP bound state, i.e., it is downregulated by its GTPase activity. Ras can transduce a signal through its effectors, which include Raf kinases, phosphoinositide 3-kinases, Ral guanine nucleotide dissociation stimulator, and phosphatases C, by the conformational change brought on by GTP binding. The conversion of GDP to GTP state and GTP to GDP state are mediated by the factors guanine nucleotide exchange factors (GEF) and GTPase activating protein (GAP), respectively. In this study, functional sites of GAP with an innovative GAP modification with the photochromic molecule of monofunctional azobenzene derivatives control GTP-GAP exchange of Ras photo-reversibly. We have designed the sites in Ras to be modified by a photochromic molecular device, azobenzene, and expressed the GAP mutant by the E. coli expression system. We have modified the GAP mutant which is S1233C. This cysteine mutant was stoichiometrically incorporated with the azobenzene derivatives N-(4-phenylazophenyl) maleimide (PAM) and Amino-azobenzene-Maleimide (AABM). The results demonstrated that the GTPase activity of Ras was controlled photo-reversibly.

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Fri/08/19

Abstract ID: 10

Importance of the Electronic Structure of Luminescent Molecules in Electrogenerated Chemiluminescence

Ryoichi ISHIMATSU, Kyushu University, Japan

The electrogenerated chemiluminescence (ECL) is a light emitting phenomenon, where the electron transfer between electrochemically generated radical anion and cation generates the excited states of luminescent molecules. Hence, the ECL involves electrode reactions, diffusion, electron transfer, and radiative electronic transition. In several cases, the interaction between the excited and ground states causes the formation of excimer and exciplex.

So far, we employed several luminescent molecules for ECL, and revealed the relation between the ECL properties with the ECL mechanism and the electronic structures of the luminescent molecules. For deep understanding of the ECL mechanism, although the electronic structure is one of the most important factors on ECL, all steps related to the ECL emission should be discussed together. In the presentation, the impact of the electronic structures and all steps, especially for the electron transfer process, on the ECL mechanism, which was recently found by us, will be introduced.

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Fri/08/19

Abstract ID: 11

On the residual stress of thermal barrier coatings

T.C. WU, XTU

Thermal barrier coatings (TBCs) based on yittria stabilized zirconia are widely used in advanced aerospace applications as high temperature thermal insulation materials. In this talk, I will be presenting research activities on characterizing interfacial residual stress, understanding coating delamination mechanisms and elucidating factors controlling thermal, micro-mechanical and physical properties of these materials.

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Sat/08/20

Abstract ID: 12

Novel Macrocycles Inspired by Natural Products

Jun O. LIU, Hanjing PENG, Zufeng GUO, Christian B. GOCKE, Brett ULLMAN, Maya THAKAR, Feiran ZHANG, Sam Y. HONG, William H. MATSUI, Johns Hopkins University, USA

Natural products have served as an invaluable source of both drugs and chemical tools to explore a wide variety of biological processes by chemical biologists. Rapamycin, FK506 and cyclosporin A (CsA) are macrocycles that have played important roles in unraveling novel cellular pathways and the treatment of organ rejection as well as other diseases. These macrocycles have a unique and extraordinary mode of action—they work by serving as molecular glues to bring two cellular proteins together to achieve the inhibition of their respective, ultimate targets, the protein phosphatase calcineurin (CsA and FK506) and mTOR (rapamycin). Inspired by the mode of action of these natural products as well as their intrinsic drug-like properties, we embarked on the design and synthesis of novel class of hybrid macrocycles known as rapafucins by replacing the mTOR-interacting effector domain of rapamycin with a combinatorial oligopeptide library. The first generation, 45,000-compound library has been synthesized and screened in a number of cell- and target-based assays. Hits against a wide variety of protein targets have been identified and characterized to date, from the SLC family of transporters including glucose transporter and non-equilibrative nucleoside transporters, the proteasome, nucleases and transcription factors. These results suggest that rapafucin has great potential as a new source of chemical probes and drug leads.

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Sat/08/20

Abstract ID: 13

Comprehensive synthesis of side-chain fluorinated vitamin D3 analogues: Construction of chemical library and exploration of drug candidates

Fumihiro KAWAGOE, Sayuri MOTOTANI, Teikyo University; Kaori YASUDA, Hiroki MANO, Toshiyuki SAKAKI, Toyama Prefecture University; Atsushi KITTAKA, Teikyo University, Japan.

Hydroxylation of vitamin D3 side-chain by human cytochrome P450 24A1 (hCYP24A1) is the deactivation pathway of both 25-hydroxyvitamin D3 and 1 ,25-dihydroxyvitamin D3 (the active form of vitamin D3). Therefore, to prolong half-life time and modulate binding affinity to vitamin D receptor, side-chain fluorinated vitamin D3 analogues have been synthesized and evaluated their biological activities. Falecalcitriol is one of such vitamin D3 analogues and contains a hexafluoroisopropanol (26,27-hexafluoro) unit on the side-chain, which is clinically approved for the treatment of secondary hyperparathyroidism in Japan.

Many efforts have been made to prepare side-chain fluorinated vitamin D3 analogues to date. However, 24,24-difluoro and 26,27-hexafluoro analogues have been mainly reported, and there are a few reports to synthesize 22-, 23-, 24-, 26- and 27-mono or difluorinated analogues even though they are catabolic sites of hCYP24A1 [24-fluoro (2 reports) and 23,23-difluoro (1 report) and 22-fluoro (1 report)].

In this research, we developed efficient stereoselective and regioselective fluorination and difluorination methods at 22-, 23-, 24-, 26- and 27-positions of the side-chain. In addition, we synthesized key intermediates of side-chain fluorinated vitamin D3 (12 side-chain fluorinated CD-rings) and constructed a chemical library of side-chain fluorinated vitamin D3 (36 analogues). We also evaluated their VDR binding affinity and hCYP24A1-dependent catabolism and revealed that their biological activities vary greatly depending on the position and stereochemistry of the fluorine atom(s).

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Sat/08/20

Abstract ID: 14

Design of lipid nanoparticles for delivery of macromolecules

Yusuke SATO, Hokkaido University, Japan

Recent advances in biotechnology have given birth to new therapeutic modalities such as nucleic acid medicine, mRNA medicine, and genome editing technology. As these are all macromolecules which show very limited in vivo stability and cellular uptake, development of sophisticated drug delivery system (DDS) which can deliver therapeutic payloads to target tissues/cells efficiently is important for therapeutic translation of the novel therapeutic modalities. Lipid nanoparticles (LNPs) are one of the most advanced DDS and are approved in clinic as a short interfering RNA (siRNA) medicine and COVID-19 mRNA vaccines. Chemistry of ionizable lipid, one of main components in LNPs, and formulation technology are especially important for efficient and specific delivery of macromolecules in vivo. I have developed original ionizable lipid libraries and shown delivery of siRNA to hepatocytes, liver sinusoidal endothelial cells and tumor-associated macrophages, mRNA to hepatocytes and splenic dendritic cells, and CRISPR/Cas9 ribonucleoproteins (RNPs) to hepatocytes. In this presentation, I will present some of my research to date.

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Sat/08/20

Abstract ID: 15

Precise synthesis of organosilicon compounds for high-performance materials

Yumiko NAKAJIMA, Yuki NAGANAWA, National Institute of Advanced Industrial Science, Japan

The transition-metal-catalyzed hydrosilylation reaction of alkenes is one of the most important catalytic reactions in the silicon industry. In this field, intensive studies have been thus far performed in the development of base-metal catalysts due to increased emphasis on environmental sustainability. However, one big drawback remains to be overcome in this field: the limited functional group compatibility of the currently available Pt hydrosilylation catalysts in the silicon industry. This is a serious issue in the production of various silane coupling agents containing various functional groups. Given the increasing demand for the precise synthesis of various organosilicon compounds to achieve more sophisticated high-performance materials in recent years, the development of novel catalytic systems that can efficiently catalyze the hydrosilylation of olefins with various functionalities is highly desirable. In this study, we have developed a series of hydrosilylation catalysts, which can form O-, S-, or P-containing organosilicon compounds with high selectivity and high efficiency.

As an alternative pathway for the efficient synthesis of organosilicon compounds, we have recently developed transition-metal-catalyzed cross coupling reactions of chlorosilanes as cheap and widely available silicon feedstocks. Treatment of chlorosilanes with reactive organometallic reagents such as organolithium or Grignard reagents is a classical yet primary method to introduce organic substituents on the Si atom. However, the reaction has a major drawback, for example, production of stoichiometric metal wastes, difficulty in the control of product selectivity in the reaction of di- or trichlorosilanes, etc. The reactions were achieved via efficient activation of Si–Cl bond using the combination of Ni or Pd catalyst and Al Lewis acid, affording various organosilicon compounds. The details of these reactions will be introduced at the presentation.

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Sat/08/20

Abstract ID: 16

TBA

Guochao XU, Jiangnan University, China

TBA

Notes

GOLDEN ACADEMY

Sun/08/21

Abstract ID: 17

Short-Range Ordering and its Impact on Property of High-Entropy Alloys

Shuai CHEN, Institute of High Performance Computing, Singapore

High-entropy alloys (HEAs) have drawn increasing attention for their superior properties. Understanding the structure-property relations of HEAs enables rational HEA design. In this talk, we will present our research work on the short-range ordering (SRO) and its impact on mechanical and thermodynamic properties of HEAs using a combination of density functional theory, molecular dynamics and Monte Carlo. First, we will discuss the formation mechanism of SRO in HEAs, which is the chemical-affinity disparity and chemical-element exclusivity. Next, we will share our work on simultaneous enhancement of ultimate strength and ductility of HEAs via SRO. Last, we will report our findings on the effect of SRO on thermodynamic properties.

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Sun/08/21

Abstract ID: 18

Progress and Prospects of Sm-Fe-N Magnets

Tetsuji SAITO, Chiba Institute of Technology, Japan

High-performance Neodymium-iron-boron (Nd-Fe-B) magnets are applied to various advanced electromagnetic devices, including hard disk drives, electric vehicles, and medical equipment. In particular, the production of electric vehicles with Nd-Fe-B magnet motors has significantly increased, because regulations on internal combustion engines that emit large quantities of greenhouse gases have been proposed or enacted in many countries. The continuously growing demand for high-performance Nd-Fe-B magnets has raised severe concerns due to their prices and availability. Under such circumstances, the use of the relatively abundant rare-earth element Sm has focused attention on the development of permanent magnets.

It is known that the samarium-iron-nitride (Sm-Fe-N) intermetallic compound possesses magnetic properties comparable to those of the Nd2Fe14B phase. Such a Sm-Fe-N magnet has not yet appeared, however, despite the fact that more than 25 years have elapsed since the discovery of the Sm-Fe-N intermetallic compound. This is because Sm-Fe-N bulk magnets cannot be produced by the sintering of Sm-Fe-N powder due to the poor thermal properties of the powder. We have continued to study the production of the Sm-Fe-N magnets. The progress of the Sm-Fe-N magnets are discussed.

Notes

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Sun/08/21

Abstract ID: 19

New development environment based on digital materials and a case study of PM filter

Kazuhiro YAMAMOTO, Nagoya University, Japan

In recent years, vehicle emission control regulations have been tightened. As for particulate matters (PMs) such as nanoparticles emitted from automobiles, their regulations for gasoline vehicles as well as diesel have been set in Europe and Japan. Normally, a PM filter is valid to trap particles in the exhaust gas after-treatment. However, the particles emitted from gasoline vehicles are considerably smaller in diameter than those from diesel vehicles, and it is necessary to significantly improve the filtration efficiency, but the PM filter has been developed mainly based on repeated experiments, including the material design and the evaluation of final product performance. Currently, it is difficult to visualize the PM filter for fully understanding the phenomena during the filtration. It is not efficient to evaluate the filter performance only by experiments, and the innovative progress cannot be expected from the material design that may rely on conventional empirical rules based on trial and error. Therefore, the simulation technology is needed to investigate pore structures suitable for nanoparticle filtration. We call the virtual materials reproduced on the computer “digital materials”. In this presentation, we will introduce a new development environment that links simulation and experiment from the material design stage for the substrate and report a case study of for PM filter with an actual porous material.

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GOLDEN ACADEMY

Sun/08/21

Abstract ID: 20

TBA

Dangyuan LEI, City University of Hong Kong, Hong Kong

TBA

Notes

GOLDEN ACADEMY

Sun/08/21

Abstract ID: 21

TBA

Haimin YAO, The Hong Kong Polytechnic University, Hong Kong

TBA

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