

Session: Materials for energy and environment (EE)EE-O01 - EE-O05

EE-O01 (Oral)**Review of Langmuir-Blodgett films of octadecylamine: Fabrication, properties, and application**

Thi Thao Vu^{1*}, Xuan Tung Nguyen¹, Dinh Tu Bui¹, Thi Huong Giang Do¹,
Phuong Hoai Nam Nguyen¹, Duc Cuong Nguyen¹, Tuan Canh Nguyen¹, Ngoc An
Nguyen¹

¹ University of Engineering and Technology, Vietnam National University Hanoi, Hanoi,
Vietnam

* Corresponding author's e-mail: vtthao@vnu.edu.vn

Nowadays, the fabrication of hydrophobic and self-cleaning nanoscale coatings is increasing. In that trend, scientists have been interested in amine octadecylamine (ODA) - a surfactant that can create stable floating films with the desired nanostructure by the Langmuir-Blodgett method. However, to fabricate and apply ODA-based film as a different functional material, it is necessary to control the factors affecting the process of film formation and deposition. In this review paper, we discuss the influence of film forming parameters on their properties and applicability, specifically: i) Spreading solution (solvent, concentration, composition), ii) Film compression velocity, iii) Subphase (pH, solvents, presence of other compounds), iv) Film deposition methods, v) Initial surface coverage degree, vi) substrate (material and surface structure); vii) Research and application of ODA films in coating technology.

Keywords: Langmuir-Blodgett, octadecylamine, Langmuir-Schaefer, coating material

EE-O02 (Oral)

Lanthanide-based Magnetoplasmonic Probes for Highly Sensitive Aqueous Copper(II) Sensing

My-Chi Thi Nguyen, Huu-Quang Nguyen, Jaebeom Lee*

Department of Chemistry, Chungnam National University, Daejeon, 34134, Republic of Korea

* Corresponding author's e-mail: nanoleelab@cnu.ac.kr

Lanthanide complexes are widely applied in imaging and sensing owing to their unique intra-configurational 4f-4f transitions. In this work, a europium (Eu) complex Eu(dbm)₃phen (dbm: dibenzoylmethane, phen: 1,10-phenanthroline) was efficiently doped into magnetoplasmonic (MagPlas) Ag@Fe₃O₄ NPs, forming a multifunctional photoluminescence NPs with intense red-emission and good response to magnetic field. The as-synthesized MagPlas NPs greatly enhanced photoluminescence intensity and quantum yield compared to the ones without the plasmonic Ag core. Furthermore, an addition of aqueous copper(II) dramatically diminished the photoluminescence emission of the Eu-doped MagPlas NPs. This quenching effect is the result of energy transfer into non-radiative emission between the doped fluorophores and copper(II). The decrease in photoluminescence intensities showed a good log-linearity in the range of 0.005-0.1 µg/mL. Therefore, Eu-doped MagPlas NPs are potential probes for sensitive detection and quantification of Cu²⁺ in aqueous samples.

Keywords: Lanthanides, magnetoplasmonic, copper(II), sensing

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EE-O03 (Oral)

Fast synthesis of ZnO/Ag heterostructure nanoparticles for enhanced photocatalytic

Cong Doanh Sai¹, Van-Phu Vu², Viet Tuyen Nguyen¹, Nguyen Hai Pham¹, An Bang Ngac^{1*}

¹ Faculty of Physics, VNU Hanoi University of Science, 334 Nguyen Trai, Thanh Xuan, Hanoi

² School of Semiconductor and Chemical Engineering, Jeonbuk National University, Jeonju, Korea

* Corresponding author's e-mail: ngacnbang@hus.edu.vn

ZnO/Ag heterostructure nanoparticles were successfully synthesized by solution method. The crystal structure and optical properties of the samples were studied by X-ray diffraction (XRD), ultraviolet-visible absorption spectroscopy (UV-Vis), and photoluminescence (PL) equipment, respectively. Morphologies of ZnO/Ag heterostructure nanoparticles composed of ZnO nanoparticles with 30 nm diameter and silver nanoparticles decorated on surface ZnO nanoparticles were examined by scanning electron microscope (SEM). Photocatalytic of ZnO/Ag heterostructure nanoparticles was evaluated by analyzing the degradation of methylene blue under UV irradiation at room temperature. The degradation of methylene blue depends on the density of Ag nanoparticles decorated on the surface of ZnO nanoparticles. The maximum methylene blue degradation efficiency of the prepared ZnO/Ag nanoparticles is up to 99% after 60 minutes of the UV treatment.

Keywords: ZnO/Ag heterostructure; Photocatalytic; nanoparticles.

EE-O04 (Oral)

Van der Waals density functional study of NO-H₂O coadsorption on Cu(111)

Thanh N. Pham^{1*}, Y. Hamamoto^{1,2}, K. Inagaki^{1,2}, I. Hamada^{1,2}, and Y. Morikawa^{1,2,3}

¹ Department of Precision Engineering, Osaka University, 2-1 Yamada-oka, Suita, Osaka 565-0871, Japan

² Elements Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University, 1-30 Goryo-Ohara, Nishikyo-ku, Kyoto 615-8245, Japan

³ Research Center for Precision Engineering, Graduate School of Engineering, Osaka University, 2-1 Yamada-oka, Suita, Osaka 565-0871, Japan

* Corresponding author's e-mail: thanh@cp.prec.eng.osaka-u.ac.jp

Elucidating the interaction between adsorbed nitric oxide (NO) and water (H₂O) on metal surfaces is of paramount importance to uncover mechanistic details of their competitive coadsorption behavior and to guide the design of new NO_x purification catalysts under wet condition.¹ Herein, we studied coadsorption and complex formation of NO and H₂O on Cu(111) using the nonlocal van der Waals density functional method.² The energetics, adsorption geometries, and vibrational properties of several $n\text{NO}-m\text{H}_2\text{O}$ complexes ($n = 1-4$, $m = 1-3$) on Cu(111) are reported, and the relative stabilities of those complexes are compared with their respective NO and H₂O clusters on Cu(111). We find that the mixed $n\text{NO}-m\text{H}_2\text{O}$ complexes on Cu(111) are more stable than separated NO and H₂O clusters due to the attractive NO-H₂O and NO-NO interactions on the surface. The attractive NO-H₂O interaction originates mainly from the hydrogen bonding between H₂O and the negatively charged NO upon adsorption. Moreover, hydrogen bonding also induces an additional back donation process from Cu(111), further strengthening the NO-H₂O coadsorption. In addition to hydrogen bonding, the NO-NO interaction originating from $2\pi^*$ orbital hybridization further stabilizes the formation of the 4NO-3H₂O complex, which is observed in the experiment.³ Even though the hydrogen bonding strength in $n\text{NO}-m\text{H}_2\text{O}$ complexes is slightly weaker than the one in H₂O clusters, due to the saturation of hydrogen bonding and the NO-NO interaction, NO and H₂O tends to form the NO-H₂O complex on Cu(111), in agreement with experiment. Our findings shed light on the role of intermolecular interactions between NO and H₂O in the formation of the NO complex, which is important for understanding the reaction of NO in three-way catalysts.

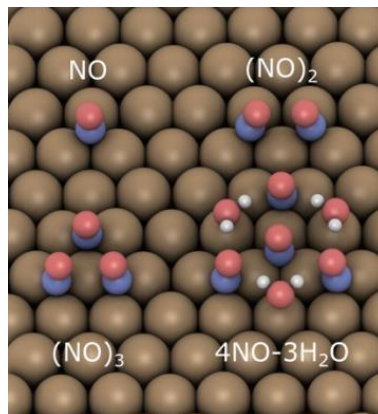


FIG. 1. Stable NO clusters and a NO-H₂O complex on Cu(111).

Keywords: NO_x catalysts, NO, H₂O, coadsorption.

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EE-O05 (Oral)

Development of high-efficient multi-layer microwave absorbers using Co-doped BaMnFe₁₁O₁₉ nanoparticles

Ngo Tran^{1,2,*}, Ruey-Bin Yang³, Bo Wha Lee⁴¹ Institute of Research and Development, Duy Tan University, Da Nang, 550000, Viet Nam² Faculty of Natural Sciences, Duy Tan University, Da Nang, 550000, Viet Nam ³

Department of Aerospace and System Engineering, Feng Chia University, Tai Chung 407, Taiwan

⁴ Department of Physics and Oxide Research Center, Hankuk University of Foreign Studies, Yongin 17035, South Korea

* Corresponding author's e-mail: tranngo@duytan.edu.vn

Co-doped BaMnFe₁₁O₁₉ (BaMn_{1-x}Co_xFe₁₁O₁₉, $x = 0, 0.4, \text{ and } 0.95$) samples were successfully prepared using co-precipitation method. XRD patterns and RS spectra confirmed M-type hexaferrite phase formation and its purity. Electromagnetic (EM) properties of the epoxied samples were modified by doping. Microwave absorption properties of epoxied samples were calculated from EM data using transmission line theory, which showed an enhancement performance for the increase of Co doping concentration. The undoped sample (BaMnFe₁₁O₁₉, named Co-0) showed a minimum reflection loss (RL) of -23.08 dB at a frequency (f) of 18 GHz for a thickness (t) of 2.25 mm. When the doping concentration increased to 0.4 (BaMn_{0.6}Co_{0.4}Fe₁₁O₁₉, named Co-4), the minimum RL achieved a value of -42.91 dB at $f = 18$ GHz with $t = 6$ mm. With higher doping concentration of $x = 0.95$ (BaMn_{0.05}Co_{0.95}Fe₁₁O₁₉, named Co-9.5), the minimum RL value bound back to the value of -37.18 dB at 10.32 GHz for a $t = 7.25$ mm. The RL values of $x = 0.4$ and 0.95 epoxied samples reached the values corresponding to $\sim 99.99\%$ of the incident microwave being absorbed. However, the t values to achieve those RL values were pretty thick. In order to enhance the microwave absorption properties with the thinner thickness of these materials, the tri-layer absorbers made from as-prepared samples were simulated for total thicknesses of 4, 5, and 6 mm. Based on the difference in layer stacking, there were six cases for each total thickness. In the case of a total thickness of 4 mm, no enhancement could be observed for tri-layer absorbers compared to single-layer ones. When the total thickness was 5 mm, the microwave absorption performance of tri-layer absorbers was significantly improved compared to single-layer ones for all six cases. In detail, the third to sixth cases slightly improved compared to single layers (the best value of RL of single layer absorbers was -18.84 dB, which was observed for Co-9.5). Notably, the first and second cases of tri-layer absorbers stacking Co-9.5/Co-4/Co-0 and Co-9.5/Co-0/Co-4 with thicknesses of 3/1/1 (mm) achieved the minimum RL of -34.85 and -36.58 dB, which is similar to the best values of single-layer ones but much thinner. In the case of tri-layer absorbers with a total thickness of 6 mm, the RL values of tri-layer absorbers could not be better than the best value of single-layer ones (achieved for $x = 0.4$ sample). However, the 6-mm-total tri-layer absorbers could reduce the absorption frequency to lower ranges, which could benefit more practical applications.

Keywords: M-type hexaferrite; Microwave absorption properties; Reflection loss; Single-layer absorber; Multi-layer absorber

Session: Multiferroics and magnetic materials (MM)

MM-O01 - MM-O07

MM-O01 (Oral)

An emergent quasi-2D metallic state derived from the Mott insulator framework

Jiunn-Yuan Lin*

Institute of Physics, National Yang Ming Chiao Tung University, Hsinchu 30010, Taiwan

* Corresponding author's e-mail: ago@nycu.edu.tw

Recent quasi-2D systems with judicious exploitation of the atomic monolayer or few-layer architecture exhibit unprecedented physical properties that challenge the conventional wisdom on condensed matter. Here we show that infinite layer SrCuO₂ (SCO), a topical cuprate Mott insulator, can manifest an unexpected metallic state in the quasi-2D limit when SCO is grown on TiO₂-terminated SrTiO₃ (STO) substrate. The sheet resistance does not conform to Landau's Fermi liquid paradigm. Hard x-ray core-level photoemission spectra demonstrated a definite Fermi level of the hole doped metal, and the soft x-ray absorption spectroscopy revealed features analogous to those of a doped Mott insulator. The key element of hole doping is not at the interfaces between SCO and STO, and likely comes from emergent transient layers between the chain-type and planar-type structures within the SCO sector as implied by an energy scan of x-ray Laue nano-diffraction. The present work emphasizes on the discovery of a new metallic state, and invites further exploration to elucidate the mysterious origin of this finding.

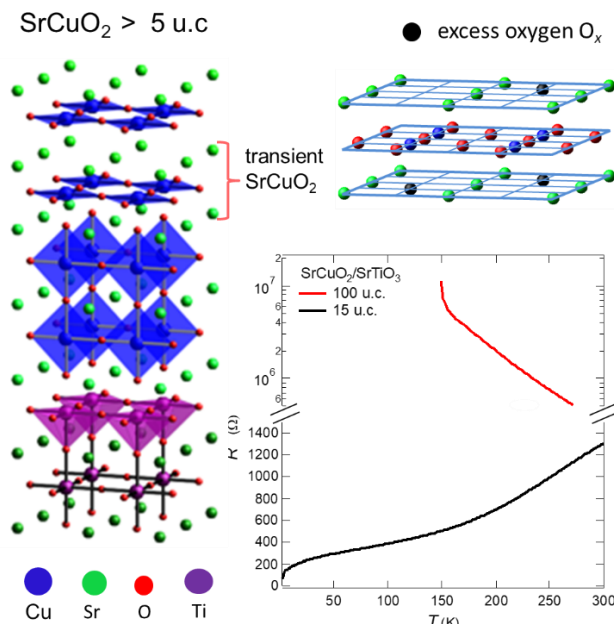


FIG. 1. The ultrathin SrCuO₂ films on SrTiO₃ become metallic.

Acknowledgments

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MM-O02 (Oral)

Deriving Maximally Orthogonalized Supercells with Given SizeYoyo Hinuma^{1,*}¹ Department of Energy and Environment, National Institute of Advanced Industrial Science and Technology, Ikeda, Osaka, Japan 563-0026

* Corresponding author's e-mail: y.hinuma@aist.go.jp

Supercells with desirable size and reasonable geometry, such as basis vectors with similar length and are close to orthogonal, are useful for defect calculations and dilute alloy calculations. However, finding supercells with given size and reasonable geometry is a non-trivial task because standard lattice reduction algorithms cannot be directly applied. I developed a computational algorithm, applicable to any crystal, that finds supercells with a certain size N with maximally and almost maximally orthogonalized basis vectors¹⁾. The list of transformation matrices converting a primitive cell to supercells with maximally and almost maximally orthogonalized basis vectors could be very long; there are 4,408,368 maximally orthogonal $N=387$ supercells of an ideal hcp lattice. One such supercell that is almost cubic is given in Fig. 1. The number of maximally orthogonalized supercells scale as roughly $O(N^2)$ at least in bcc, fcc, and sc lattices. The computational cost could be reduced to approximately $O(N^2)$ by carefully choosing basis vector lengths as $a \leq b \leq c$ and mathematically deriving upper limits to the lengths of a and b .

Using almost maximally orthogonalized basis vectors allows conversion of basis vectors in similar crystals with very different crystallographic conventional basis vectors, such as NASICON-type structure $\text{Ag}_3\text{Sc}_2(\text{PO}_4)_3$. The algorithm is also useful in converting different basis vector choices in energy application-related materials, LiCoO_2 , and Li_2MnO_3 .

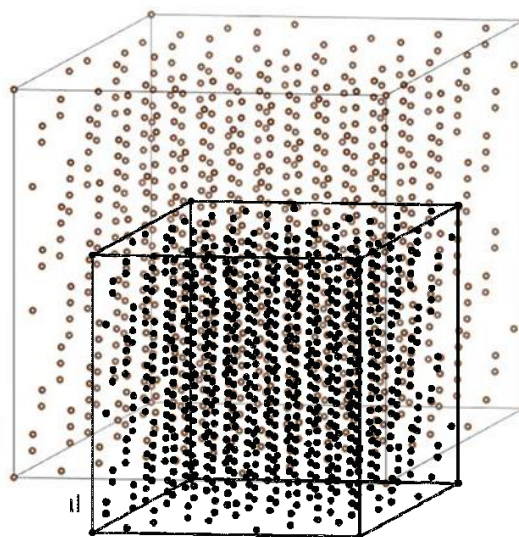


FIG. 1. 387-supercell of an ideal hcp lattice that is almost cubic.

Keywords: Supercell, maximally orthogonalized, basis vectors, algorithm**References**

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MM-O03 (Oral)

Bayesian Optimization Design of High Entropy Oxide for Oxygen Evolution Catalysis

Yuichi Okazaki¹, Yushi Fujita¹, Hidenobu Murata¹, Naoki Masuyama², Yusuke Nojima², Hidekazu Ikeno¹, Ikuya Yamada¹, and Shunsuke Yagi³

¹ Graduate School of Engineering, Osaka Metropolitan University, Sakai, Osaka 599-8531, Japan

² Graduate School of Informatics, Osaka Metropolitan University, Sakai, Osaka 599-8531, Japan ³Institute of Industrial Science, The University of Tokyo, Tokyo 153-8505, Japan

* Corresponding author's e-mail: ikuya_yamada@omu.ac.jp

High entropy oxides (HEOs), containing five or more kinds of mixed metals, have been investigated as highly active oxygen evolution reaction (OER) catalysts [1]. Recently, it was reported that the Co-enriched perovskite oxide of $\text{LaCr}_{1/6}\text{Mn}_{1/6}\text{Fe}_{1/6}\text{Co}_{1/3}\text{Ni}_{1/6}\text{O}_3$ ($\text{M}_{1/6}\text{Co}_{1/3}$) exhibited a higher activity than that with equimolar 3d transition metals ($\text{LaCr}_{1/5}\text{Mn}_{1/5}\text{Fe}_{1/5}\text{Co}_{1/5}\text{Ni}_{1/5}\text{O}_3$: $\text{M}_{1/5}$) [2]. This enhancement indicates that the chemical compositions of HEOs play a crucial role in OER catalytic activities, whereas the vast composition space of HEOs prevents the optimization by experiments. In this study, we performed Bayesian optimizations to achieve the highly active catalysts in the $\text{La}(\text{Cr},\text{Mn},\text{Fe},\text{Co},\text{Ni})\text{O}_3$ HEOs. We conducted three cycles of experiments (synthesis, phase identifications, and electrochemical characterization) via Bayesian optimization using the initial composition–activity dataset of references and HEOs with random compositions (R- HEOs). The data of HEOs with the compositions determined by Bayesian optimizations (BO-HEOs) were added to the dataset in the respective cycles. All the R- and BO-HEOs crystallized in orthorhombic and rhombohedral perovskite-type structures. OER catalytic activities (A_{OER}) in 0.1M KOH solution were evaluated using the rotating disk electrode system described in the reference [3]. The average A_{OER} of BO-HEOs [0.14(6) mA cm^{-2} in BO_{ave}] was larger than that of R-HEOs [0.04(2) mA cm^{-2} in R_{ave}], as displayed in Fig. 1. The A_{OER} of BO-HEOs were larger than or comparable to that of $\text{M}_{1/5}$ with a high probability, differing from lower activities in most of R-HEOs. Consequently, we propose that the Bayesian optimization is a useful way to adjust the chemical compositions for highly active HEO in the limited number of trials.

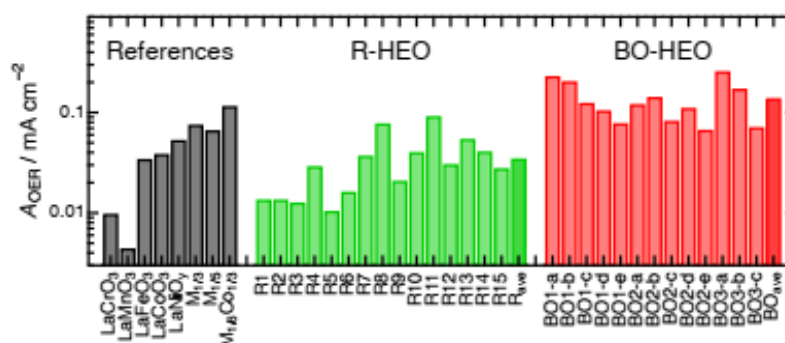


FIG. 1 OER activities (A_{OER}) for references (black), R-HEOs (green), and BO-HEOs (red), together with their average values of R_{ave} and BO_{ave} .

Keywords: oxygen evolution reaction catalyst, Bayesian optimization, high-entropy oxide

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MM-O04 (Oral)

Magnetocaloric effect from first-principles calculations and Monte Carlo simulationsHung Ba Tran^{1,2*}, Yu-ichiro Matsushita^{1,2,3}¹ Institute of Innovative Research, Tokyo Institute of Technology, Tokyo, 152-8550, Japan² Quemix Inc., Taiyo life Nihombashi Building, Tokyo, 103-0027, Japan³ Quantum Material and Applications Research Center, National Institutes for Quantum Science and Technology, Tokyo, 152-8552, Japan

* Corresponding author's e-mail: tran.h.ag@m.titech.ac.jp

Sustainable energy, which utilizes clean and affordable energy, becomes essential to sustainable development goals (SDGs). One of the most energy consumption parts for many developed and developing countries is cooling and heating energy due to global warming and climate change. Traditional cooling and heating method is harmful to the environment due to the use of greenhouse gas, which will be banned in Europe and other countries shortly. The magnetocaloric effect, as the intrinsic property of magnetic material, is a promising candidate for future cooling devices. This work studies the magnetocaloric effect of several well-known materials by combining first-principles calculations and Monte Carlo simulations [1,3]. All parameters for the simulations, such as isotropic exchange coupling constant (J_{ij}), Dzyaloshinskii-Moriya interactions (D_{ij}), and magnetocrystalline anisotropy energy (MAE), are estimated from first-principles calculations based on density functional theory. Temperature-dependent of magnetocrystalline anisotropy energy is quantitatively reproduced by considering the magnetization-magnetic field ($M-H$) integration in Monte Carlo simulations. In addition, the isothermal magnetic entropy change is calculated by the Maxwell relation, which is discussed and compared with experimental works in detail.

Keywords: Isothermal magnetic entropy change, Density functional theory, Monte Carlo simulations.

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MM-O05 (Oral)

Synthesis of bifunctional magnetic-plasmonic Fe₃O₄@SiO₂-Au nanoparticles by an ultrasound assisted chemical method

Phi Thi Huong^{1,2,*}, Bui Duc Tri³, Nguyen Thị Thanh Van⁴, Tran Thi Hong⁵, Luu Manh Quynh¹, Nguyen Hoang Luong^{2,3}, Nguyen Hoang Nam^{2,3,*}

¹ Faculty of Physics, VNU University of Science, Hanoi, Viet Nam

² Nano and Energy Center, VNU University of Science, Hanoi, Viet Nam

³ Master Program in Nanotechnology, VNU Vietnam Japan University, Hanoi, Viet Nam

⁴ Vietnam Academy of Cryptography Techniques, Hanoi, Viet Nam

⁵ Faculty of Environmental Sciences, VNU University of Science, Hanoi, Viet Nam

* Corresponding author's e-mail: phithihuong@hus.edu.vn, namnh@hus.edu.vn

Bifunctional magnetic-plasmonic nanoparticles Fe₃O₄@SiO₂-Au (FSAs) were successfully synthesized by an ultrasound assisted chemical method. Gold ions were absorbed on the surface of 3-aminopropyltriethoxysilane (APTES)-functionalized silica-coated magnetic nanoparticles and then reduced by sodium borohydride (NaBH₄) under the influence of a 200 W ultrasonic wave for 45 min. The composed FSAs exhibit superparamagnetism with high saturation magnetization and simultaneously absorb visible blue light with the surface plasmon resonant (SPR) peak at around 545 nm. When the amount of precursor gold ions increased from 16 μmol to 40 μmol, the relative the atomic ratio of gold/iron increasing from 0.84 to 3.35, likewise the peak absorption positions increased from 540 nm to 550 nm regarding to the increase of the Au crystal size. The controllable magnetic and absorption properties of the particles make the particles become a reasonable for wide range of bio-application, such as MIR imaging, magnetophoretically-enhanced photothermal therapy, etc.

Keywords: Bifunctional nanoparticles, magnetic-plasmonic, ultrasound assisted chemical method.

MM-O06 (Oral)

Thermal evaporation synthesis and some properties of WO₃/ITO electrochromic thin films

Nguyen Duy Thien¹, Nguyen Quang Hoa¹, Vuong Van Hiep¹, Le Van Vu¹, Hoang Nam Nhat², Nguyen Ngoc Dinh^{1*}

¹ Faculty of Physics, University of Science, Vietnam National University, Hanoi, 334 Nguyen Trai, Thanh Xuan, Hanoi, Vietnam

² Faculty of Engineering and Nanotechnology, VNU-University of Engineering and Technology, 144 Xuan Thuy, Cau Giay, Ha Noi, Vietnam

* Corresponding author's e-mail: nguyennngocdinh@hus.edu.vn

This paper reports the results of thermal evaporation synthesis and properties of WO₃/ITO electrochromic thin films. The influence of annealing temperature on the crystal structure and Raman scattering spectrum of WO₃/ITO thin films were investigated in detail by X-ray diffraction (XRD) and Raman scattering spectroscopy. The results shown that thin films annealed at 400 °C and 500 °C have crystallized in triclinic, film is quite smooth, with surface roughness of only 4 nm. The electrochromic characteristics investigation of WO₃/ITO thin films shown that them have a high transmittance of about 92 % in the visible wavelength region from 400 to 900 nm, good substrate adhesion. The transmittance of WO₃ thin film was reduced to around 2% in visible region when increasing the coloration time from 0 s to 90 s at applied voltage of 0.7 V. The transmittance of the film was recovered to 85 % by using an applied voltage of 0.7 in time of 150 s. The change in the optical bandgap of WO₃/ITO thin films in the coloration process were observed.

Keywords: Electrochromic, electrochemical, WO₃, thin film, thermal evaporation.

MM-O07 (Oral)

Fabrication of RuO₂ thin film for spin orbit torque – induced magnetization switching

Nguyen Thi Van Anh^{1,2,*}, Vu Duong³

¹ Center for Science and Innovation Spintronics (Core Research Cluster), Tohoku University, Japan

² Center for Innovative Integrated Electronic Systems, Tohoku University, Japan

³ Institute of Physics, Vietnam Academy of Science and Technology, Hanoi, Vietnam

* Corresponding author's e-mail: nguyen.thi.van.anh.e7@tohoku.ac.jp

Transition metal oxide RuO₂ is widely used in electrochemical reactions, as well as in electrical applications thanks to its peculiar properties such as low resistivity, chemical stability, and so on [1]. Especially, some recent studies have reported the high-temperature antiferromagnetic properties, the Dirac nodal semimetal, or the spin-split effect in RuO₂ film [2], making it attractive for spintronic device applications. We recently reported spin-orbit torque-induced magnetization switching in a RuO₂-based stacking structure [3]. However, a detailed investigation of the crystallinity is lacking. Herein, we report the fabrication of RuO₂ films and analyze their crystallinity and their Raman spectroscopy in detail.

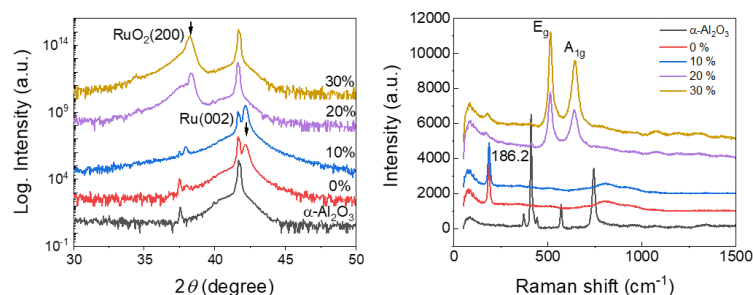


Fig. 1: (a) XRD 2θ - θ patterns and (b) Raman spectra of Ru-O films prepared at different ratio of Oxygen gas.

RuO₂ thin film was fabricated on an α -Al₂O₃ (0001) substrate by reactive sputtering at 300°C with a mixture of O₂ gas and Ar gas at different ratios of O₂ gas (P_{O_2}). Figure 1 (a) shows the X-ray diffraction (XRD) patterns of Ru-(O) films at different P_{O_2} . As $P_{O_2} \leq 10\%$, only Ru(002) peak was observed. As $P_{O_2} \geq 20\%$, only RuO₂(200) peak was observed, indicating the formation of the (100)-oriented RuO₂ film. Figure 1 (b) shows the Raman spectra of Ru-O films at different P_{O_2} . Only one peak at 186.2 cm⁻¹ was observed for films prepared at $P_{O_2} \leq 10\%$, which can be attributed to the Ru-Ru stretching vibration in a Ru film [4]. At $P_{O_2} \geq 20\%$, two phonon modes in RuO₂ were observed at 513.2 cm⁻¹ (E_g) and 644.8 cm⁻¹ (A_{1g}) [5]. Using the RuO₂ film prepared at $P_{O_2} = 30\%$, we observed the spin-orbit torque-induced magnetization switching in a RuO₂/Co-Fe-B bilayer. More details will be discussed in the presentation.

Keywords: Transition metal oxide, Rutile, spin-orbit torque, RuO₂.

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Session: Photonics and Hybrid Materials (PH)PH-O01 - PH-O05

PH-O01 (Oral) (Cancelled)**Optoelectronic and vibrational properties of Nitrogen-doped hexagonal graphene quantum dots**Minh Triet Dang^{1*}, Pham Vu Nhat², Van An Dinh³¹ School of Education, Can Tho University, Cantho, Vietnam² Department of Chemistry, Can Tho University, Cantho, Vietnam⁴ Department of Precision Engineering, Osaka University, Osaka, Japan

* Corresponding author's e-mail: dmtriet@ctu.edu.vn

Graphene quantum dots have been widely studied recently thanks to its unique optical, electrical and optoelectrical properties in applications in solar devices. Here, we investigate the optoelectronic and molecular vibrational properties of hexagonal graphene quantum dots and nitrogen doped graphene quantum dots using first principles method. We have shown that by doping a Nitrogen atom to hexagonal graphene quantum dots, the optical absorption of quantum dots is red-shifted towards the visible light range compared to that of the pristine graphene quantum dots, and the doped Nitrogen atom introduces a clear signature of anisotropy of the absorption spectrum. More interestingly, the absorption peaks predicted by time dependent density functional theory show excellent agreement to those of the experimental observations. These results highlight a novel approach of bottoming up the next generation of solar devices with assembled quantum dots to improve their light selectivity as well as efficiency.

Keywords: Nitrogen-doped graphene quantum dots, optoelectronic properties, density functional theory

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PH-O02 (Oral)

Preparation of Nanoparticulate WO_3/MoO_3 Films for Making Electrochromic Devices

Chia-Chun Wei, Tung-Han Wu, Wen-Bin Jian*

Department of Electrophysics, National Yang Ming Chiao Tung University, 1001 University Road, Hsinchu 30010, Taiwan

* Corresponding author's e-mail: wbjian@nycu.edu.tw

Sustainable and green technologies of electro-exploding wire and spray coating were employed for the deposition of nanoparticulate WO_3/MoO_3 films. The WO_3 and MoO_3 nanoparticles were characterized by TEM and AFM and the spray-coated nanoparticulate films were inspected using XRD and Raman spectroscopy. The films were immersed in electrolyte in a potentiostat for current-voltage measurements to obtain the diffusion coefficients, stored charge densities, transmittance, and electrochromic switching time. Finally, optical performances of electrochromic devices (ECDs) based on nanoparticulate WO_3/MoO_3 films were measured. Our results presented an enhancement of violet and ultraviolet switching after introduction of MoO_3 into WO_3 films.

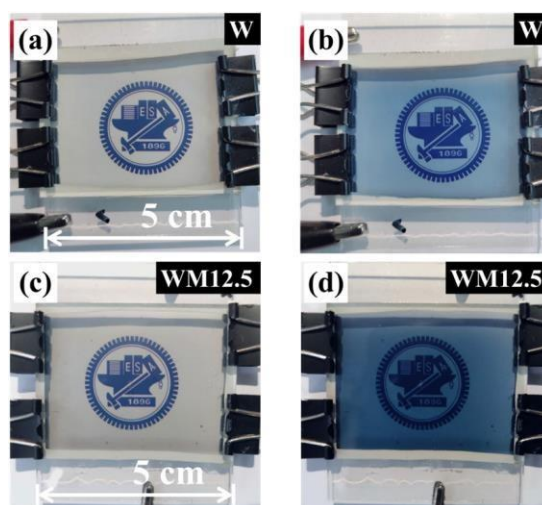


FIG. 1. (a) and (b) are photographs of colored and bleached state of ECD based on nanoparticulate WO_3 films that are driven at -3.3 V and 2 V, respectively, for 20 s. (c) and (d) are photographs of colored and bleached state of ECD based on nanoparticulate $(\text{WO}_3)_{0.875}(\text{MoO}_3)_{0.125}$ films.

Keywords: Electrochromic Devices, Tungsten Trioxides, Molybdenum Trioxides, Nanoparticle Composites

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PH-O03 (Oral)

Studying Defects in TMD Materials and Devices by STM

Chun-Liang Lin*

Department of Electrophysics, National Yang Ming Chiao Tung University, Hsinchu, Taiwan

* Corresponding author's e-mail: clin@nycu.edu.tw

Transition metal dichalcogenide (TMD) materials with ultrathin thickness provide a promising solution to scale down current semiconductor devices. Many studies have demonstrated that molybdenum disulfide (MoS_2) is able to fabricate field-effect transistors (FETs). However, the carrier mobility in MoS_2 FET is usually lower than the theoretical prediction. Although this poor performance can be attributed to the defects, it still lacks a quantitative analysis clarifying the correlation between carrier mobility and defect density. By using scanning tunneling microscopy (STM), we directly counted the defects in MoS_2 FETs with different carrier mobility. It's found that vacancies and impurities equally contribute to carrier mobility and the total defect density induces a power-law decreasing tendency to the carrier mobility of MoS_2 FET. Therefore, it urgently requires a method to eliminate defects in TMD materials. Here, a counterintuitive approach to eliminating surface defects on TMD materials is found. It's a two-step process including Ar ion bombardment and subsequent annealing. By using STM, it's proved that the defects on the *in-situ* cleaved TMDs surfaces were decreased by more than 99% after ion bombardment and subsequent annealing.

Keywords: transition metal dichalcogenide (TMD), scanning tunneling microscopy (STM), defects, carrier mobility

PH-O04 (Oral)**Abnormal Spectral Shift of Surface Plasmon Resonance**Heongkyu Ju ^{1,*}, Saikiran Kosame ¹, Than Thi Nguyen ¹, and Jun-Ho Lee ²¹ Department of Physics, Gachon University, Seongnam-si, 13120, Republic of Korea² Laser& Opto-electronics Team, Korea Electronics Technology Institute (KETI), Seongnam-si, 13509, Republic of Korea

* Corresponding author's e-mail: batu@gachon.ac.kr

We experimentally demonstrated the spectral blue shift of surface plasmon resonance due to coupling of plasmons with photo-induced excited emitters. Such spectral blue shifts that are in contrast to red shifts widely witnessed in surface plasmon spectroscopy [1-2], could be demonstrated in either linear or nonlinear regime of light matter interactions.

First, the linear interaction for such abnormal spectral shift took place by plasmons-excited quantum dots coupling in a plasmonic nanofilm coated optical fibers [3-5]. Experimental observations were interpreted using the theoretical modelling with the Kramers-Kronig (KK) relation at the visible wavelength of light. The blue shift observed could be interpreted as resulting from excited quantum dots coupling with plasmons whereby the KK relation could predict the negative local refractive index near plasmons [6-7]. Second, the abnormal blue shift of plasmon resonance was also obtained in a nonlinear interaction of light where indigo carmine (an organic dye) acted as a nonlinear medium that simultaneously coupled with plasmons. The third-order optical nonlinearity for the self-defocusing negative refractive index induced by indigo carmine at plasmon resonant wavelengths accounted for such spectral blue shift. We provided discussion on the experimental results with theoretical interpretations using energy structures of indigo carmine for applications possibly found in optical limiting technologies.

Keywords: plasmon resonance, spectral blue shift, quantum dot, nonlinearity, negative refractive index

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PH-O05 (Oral)

Electronics and Optoelectronics of Atomically Thin Semiconductors

Der-Hsien Lien *

Institute of Electronics, National Yang Ming Chiao Tung University, Hsinchu, Taiwan

* Corresponding author's e-mail: dhlien@nycu.edu.tw

Ultrathin semiconductors, such as 2D transition-metal dichalcogenide (TMDC) and < 2 nm-thick oxide semiconductors (OS), have drawn significant attention in the past decade due to their promising device performance and profound physics. 2D TMDC provides an ideal platform to investigate the photophysics of excitons and their complexes. Such 2D excitonic systems are promising for optoelectronic applications. The monolayer of 2D TMDC shows near-unity photoluminescence (PL) quantum yields (QYs), a key metric dictating the maximum efficiency as using the material for light-emitting diodes, lasers, and solar cells applications. I will discuss the recombination mechanisms of excitons in monolayers and show that the non-radiative recombination pathways can be fully suppressed by electrostatic gating, despite the presence of native defects. This result reveals that room-temperature excitons are robust and bright regardless of monolayer quality, indicating the potential of achieving highly efficient excitonic devices. Ultrathin OS is regarded as potential channels materials for FETs as they exhibit high carrier mobilities and high on/off ratio. I will show the degree of freedom to engineering transport characteristics of the OS transistors. I will show that precise control over V_T assists in realizing complex integrated systems that requires extensive manipulation of operating conditions.

Keywords: 2D semiconductors, transition metal dichalcogenide (TMD), exciton physics, oxide semiconductors, transistors.

Session: Spintronic materials and devices (SD)SD-O01 -SD-O07

SD-O01 (Oral)**Solid-liquid structure of Cu₂S: Theoretical acanthite-like model forelectronic and transport properties investigations**Ho Ngoc Nam^{1,2*}, Katsuhiko Suzuki², Akira Masago³, Tien Quang Nguyen², Hikari Shinya^{3,4,5}, Tetsuya Fukushima^{3,6,7}, and Kazunori Sato^{2,3}¹ Department of Precision Science and Technology, GSE-Osaka University, Osaka 565-0871, Japan² Division of Materials and Manufacturing Science, GSE-Osaka University, Osaka 565-0871, Japan³ Center for Spintronics Research Network, GSES-Osaka University, Osaka 560-8531, Japan⁴ Research Institute of Electrical Communication, Tohoku University, Miyagi 980-8577, Japan⁵ Center for Spintronics Research Network, Tohoku University, Sendai, Miyagi 980-8577, Japan⁶ Institute of Solid State Physics, The University of Tokyo, Chiba 277-8581, Japan⁷ Institute for AI and Beyond, The University of Tokyo, Bunkyo-ku, Tokyo 113-8656, Japan

* Corresponding author's e-mail: honam@mat.eng.osaka-u.ac.jp

Ideas of compact, wearable, and environmentally friendly personal electronic devices that are capable of self-charging using human body temperature have become more feasible in recent years. However, the development of this technology strongly depends on thermoelectric (TE) material that must have ductility and high TE performance at low temperatures [1]. Recently, experimental work uncovered the extraordinary ductility of the inorganic semiconductor Ag₂S [2], potentially paving the way for developing flexible TE devices. In this work, the electronic and transport properties of Cu₂S, a promising candidate for flexible TE application are theoretically elucidated by using first-principles calculations combined with the Boltzmann transport equation [3]. The interesting properties of Cu₂S are mainly driven by the liquid-like behavior of the Cu atoms, which is also a barrier that confuses us in determining their atomic positions and electronic properties. Using a theoretical model driven from a similar low-temperature phase of Ag₂S called the acanthite-like phase, we confirm the appearance of electronic structure with the indirect bandgap of 0.9-0.95 eV as observed in the experiment [4]. In addition, the use of the electron-phonon scattering approximation allows us to estimate the electron energy relaxation time, thereby reproducing the reasonable results of transport property compared to experimental observation. Therefore, demonstrates that the acanthite-like model is ideally suitable and can be used for TE material design related to the low-temperature phase of Cu₂S.

Keywords: electronic structures, transport properties, electron-phonon coupling, flexible thermoelectrics.

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SD-O02 (Oral)**Graphene supported liquid crystal phase retarders on rigid glass and flexible polydimethylsiloxane substrates**Stefan Petrov¹, Vera Marinova^{1,2} and Shiuan Huei Lin^{1*}¹ Department of Electrophysics, National Yang Ming Chiao Tung University, Hsinchu 30010, Taiwan² Institute of Optical Materials and Technologies, Bulgarian Academy of Sciences, Sofia 1113, Bulgaria

* Corresponding author's e-mail: lin@nycu.edu.tw

To implement unique functionality of graphene into Liquid Crystal (LC) enable devices for practical applications, the key challenge is still encountered to have a large scale (inches-by inches) high-quality graphene offering low sheet resistance and high optical transmittance as well as high precise alignment of LC molecules on the top of the graphene surface. In this paper, we demonstrate functionality of multilayer graphene, grown by atmospheric pressure CVD method, to support large surface area (inch-scale) tunable LC phase retarders on rigid glass and flexible polydimethylsiloxane (PDMS) substrates. We first focused on important steps during fabrication process of LC structures based on a detailed investigation of interfacial interaction between graphene/LC molecules by considering graphene's surface free energy as well as proper selection of polyamide (PI) as a polar layer for a non-contact planar alignment of LC molecules. A non-contact planar alignment of LC molecules instead of mechanical rubbing technique enables prevention of graphene de-attachment from the target substrate. Moreover, multilayer graphene shows excellent wettability when contacting with the polyamide. Measured electro-optical characteristics, such as voltage-dependent transmittance, response time and electrically tunable phase modulation of fabricated LC phase retarders reveal completely equivalent performance of LC retarders using conventional ITO contacts. Besides excellent phase modulation repeatability over the large scale area of the retrofitted LC structure, we demonstrate an electrically tunable LC phase retarder supported by graphene on PDMS that exhibits great potential for future ITO-free LC photonic devices and bio-oriented technologies. We also expect these demonstrations are relevant to use in high-end optoelectronics and would provide a significant step in fabricating tunable graphene-based LC components for flexible and stretchable optoelectronics.

Keywords: multilayer graphene, ITO-free liquid crystal photonic device, flexible photonic device.

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SD-O03 (Oral)

Advantages, Challenges and Opportunities of X-ray Absorption Spectroscopy for Advanced Investigation of Energy Materials

Chung-Li Dong^{1,*}

¹ Department of Physics, Tamkang University, Tamsui 25137, Taiwan

* Corresponding author's e-mail: cldong@mail.tku.edu.tw

The materials scientists are devoted to searching for sustainable and clean energy in response to the global surge in demand for energy. It has never been easy to be green without developing advanced renewable energy materials. We have to approach the zero-emission future from different angles. The universal emphasis on energy is to develop advanced functional materials for more efficient energy conversion, storage, and conservation. The concepts to improve the energy conversion, storage or conservation efficiency of current energy materials are simple and clear, but are always much technically challenging. Most of the physical and chemical properties of a material is closely related to its unique atomic and electronic structures. Hence, without knowing the fundamental atomic and electronic structures, and particularly how they response in its working condition, it is difficult to better engineer the materials in an efficient way for a practical use with a greater performance. Synchrotron x-ray spectroscopies, including x-ray absorption and x-ray emission spectroscopies are powerful tools to study the local unoccupied and occupied electronic states. Moreover, utilization of the in situ technique that gives us the opportunity to track the modulations of atomic and electronic structures of the energy material at work. The emerging x-ray spectro-microscopic approach, scanning transmission x-ray microscopy providing the spatially resolved x-ray spectroscopy, is also gearing up for energy science. This presentation will report the significances of using x-ray spectroscopies for atomic and electronic structure characterizations of several important energy material systems, such as artificial photosynthesis materials, advanced nanocatalysts, and smart materials. Emerging characterization tool, recent progress of in situ technique development, a number of recent studies and Tamkang University (TKU) end-stations recently constructed at the Taiwan Photon Source (TPS) 45A & 27A beamlines for energy science will also be presented.

Keywords: X-ray absorption spectroscopy, energy materials, atomic and electronic structures, in situ x-ray absorption spectroscopy

SD-O04 (Oral)

Fabricate electrospun nanofiber for rechargeable batteries

Nguyen Tuan Canh^{1,*}, Nguyen Phuong Hoai Nam¹, Nguyen Duc Cuong¹, Vu Thi Thao¹, Bui Dinh Tu¹

¹ Faculty of Engineering Physics and Nanotechnology, VNU-UET, Hanoi, Vietnam

* Corresponding author's e-mail: canhnt@vnu.edu.vn

Nanofibers produced by sol-gel electrospinning show an interlaced and highly porous structure with a large surface-to-volume ratio. Such property makes the nanofibers useful in several applications such as healthcare, food packaging, biotechnology, environmental engineering, defense & security, rechargeable, and energy storage. In this study, an Electrospinning system fabricated polyvinyl alcohol (PVA) nanofibers as a mock-up separator in the lithium metal battery. By varying the PVA: DI water ratio by mass, nanofibers were obtained by manipulating various parameters of electrospinning: applied voltage, flow speed, working distance, and spinning time. The ratio of PVA in DI water was found to affect the electrospinnability, fiber morphology, and diameter of fibers. The highly-porous nanofibrous structure was observed by a scanning electron microscope (SEM), and the physical properties were analyzed including porosity, toughness, and heat resistance.

Keywords: Electrospinning, nanofiber, PVA, separator

SD-O05 (Oral)**Is it possible to electropolish tungsten carbides?**

Minh Nhat Dang¹, Surinder Singh¹, Thomas G. Pattison¹, Hoang Le², Rosalie Hocking¹, Scott A. Wade¹, Guy Stephens³, Angelo Papageorgiou³, Hong Tuan Nguyen⁴, James Wang^{1,*}

¹ Australian Research Council (ARC) Industrial Transformation Training Centre in Surface Engineering for Advanced Materials (SEAM), School of Engineering, Swinburne University of Technology, Hawthorn VIC 3122, Australia

² The Electron Microscopy And Materials Analysis Research Group, School of Computing and Engineering, University of Huddersfield, Queensgate, Huddersfield HD1 3DH, United Kingdom

³ Sutton Tools, 378 Settlement Rd, Thomastown VIC 3074, Australia

⁴ Centre for Advanced Materials Technology Development, Centre for High Technology Development, Vietnam Academy of Science and Technology (VAST), 18 Hoang Quoc Viet, Hanoi 100000, Vietnam

* Corresponding author's e-mails: nhatminh@swin.edu.au & jawang@swin.edu.au

Tungsten carbide (WC) based alloys are widely used in cutting tools due to their superior tensile strength, compression strength stiffness, and wear resistance, compared to other carbide based alloys. The addition of cobalt as a primary binder improves the overall strength of the material. For cutting tools not only are the substrate properties important, but the geometry, cutting edge profile, and surface finish are also critical to the performance and working life of the tool. A high quality surface finish and cutting edge preparation can improve the service life of the cutting tools. Chemical methods of surface treatment can offer an even surface finish to geometrically complex substrates such as drill bits which are challenging to finish evenly using physical techniques. Compared to etching and electrical discharge machining, electropolishing offers tailorability over the surface finishing process, resulting in a high degree of control over material removal. This process can produce surfaces with very low surface roughness ($S_a > 100$ nm), maintaining edge geometries of the tool. This talk will discuss the potential for electropolishing to provide a high quality finish to WC substrates, and in particular the challenges to be considered when applying chemical polishing techniques to WC-Co surfaces

Keywords: electropolishing, cutting tools, tungsten carbide, cobalt leeching, edge preparation

SD-O06 (Oral)**Tandem cyclooxidative reaction of anthranilamide and alcohols over Fe(III)-based MOFs: effect of structure on catalytic efficiency**Tan Le Hoang Doan^{1*}¹ Center for Innovative Materials and Architectures, Vietnam National University Ho Chi Minh City

* Corresponding author's email: dlhtan@inomar.edu.vn

Metal-organic frameworks (MOFs), porous crystalline materials, have emerged as promising heterogeneous catalysts in organic transformations. In this research, triangular Fe(III) cluster-based MOFs were highly efficient heterogeneous catalysts for the solvent-free one-pot reaction of 2-aminobenzamide and alcohols to synthesize quinazolin-4-ones under microwave irradiation. The catalytic properties of the Fe-MOFs ranging from microporous to mesoporous structures with the various geometrical pore structures were investigated. Owing the opening accessible spaces for reactants and high density of active sites, MOF-907, built from trimmer Fe clusters and a mixture of two linkers, was more effective than other Fe(III)-MOFs. The catalyst can be used in a broad substrate scope and recycled several times without losing its structure and activity.

Keywords: Metal-organic frameworks, Heterogeneous catalyst, Solvent-free, Microwave irradiation

SD-O07 (Oral)

Nanowire Single Crystal Grain Field Effect Transistors and Their Applications

Thi Thuy Nguyen^{1,2}, Tatsuaki Hirata¹, and Shin-Ichiro Kuroki¹¹Research Institute for Nanodevices, Hiroshima University, Hiroshima 739-8527, Japan.²Faculty of Physics, Hanoi National University of Education, Ha Noi, Vietnam.

Email: nguyenthuy@hnue.edu.vn

Single crystal grain (s-G) field effect transistors (FETs) have been the key target for their large electronic applications such as monolithic three-dimensional integrated circuits (3DICs), and glass sheet computers. Highly (110)-(111)-(211) and (100) biaxial-oriented poly-Si thin films have been realized by multiline beam continuous-wave laser lateral crystallization (MLB-CLC) with very long crystal grains.[1, 2] By aligning TFTs' channels to elongate the longitudinal crystal grains, s-G FETs were fabricated at a low temperature process of below 550°C with nanowire Si channels.

Figure 1 shows the I_D and μ_{ef} versus V_G curves at $V_D = 0.5$ V of a nanowire s-G FET of 220 nm width. It indicates that this transistor had an ultrahigh performance with an electron field effect mobility of 1360 cm^2/Vs , an ON/OFF ratio of 10^7 - 10^8 , subthreshold slope (S) of 0.17 V/dec, a threshold voltage (V_{th}) of -0.5 V. This performance enhancement was brought about by the uniaxial tensile strain in the poly-Si thin film.

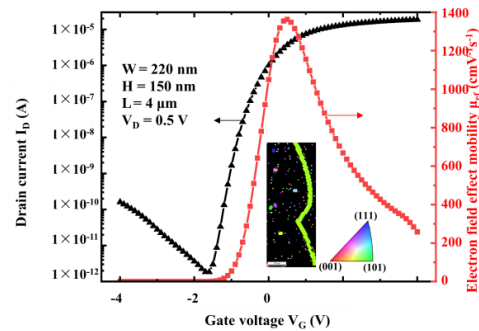


FIG. 1. I_D and μ_{ef} versus V_G curves of a nanowire s-G FET.

Acknowledgments

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Session: Theory and computation (TC)

TC-O01 - TC-O02

TC-O01 (Oral)

The first-principles analysis of Multiplet excitations using QSGW

Katsuhiro Suzuki^{1,*}, Takao Kotani^{2,3}, Kazunori Sato^{1,2,4}

¹ Graduate School of Engineering, Osaka University, Osaka 565-0871, Japan

² CSRN-Osaka, Osaka University, Osaka 560-8531, Japan

³ Department of Applied Mathematics and Physics, Tottori University, Tottori, 680-8552, Japan

⁴ Spintronics Research Network Division, OTRI, Osaka University, Osaka, 565-0871, Japan

* Corresponding author's e-mail: k-suzuki@mat.eng.osaka-u.ac.jp

The photoluminescence of rare-earth atoms is one of the important phenomena in strongly correlated electron systems. In these phenomena, the multiplet transitions of $4f$ orbitals are important. However, it is difficult for analyzing from the first-principles calculation. Traditionally, the model-Hamiltonian methods based on the atomic multiplet theory have been developed to explain the photoluminescence spectra of rare-earth atoms. These theories have empirical parameters to reproduce experiments. Therefore, the application of computational material design is difficult. On the other hand, the first-principles calculation can be applied for hypothetical structure, but we cannot discuss multiplet excitations directly.

In this study, we try to obtain excitation of the f -orbitals system from the first-principles calculation. Generally, it is known that DFT calculation with LDA/GGA functional underestimates electron correlations. Thus, we use quasi-particle self-consistent GW (QSGW) approximation[1] to consider more accurate correlations. After that, we estimate the parameters of the model Hamiltonian so that the band structure from QSGW reproduces the local atom model Hamiltonian applied mean-field approximation.[2] Figure 1 shows the QSGW band structure of free Eu ion and onsite energy of model Hamiltonian. It shows that the mean-field model Hamiltonian reproduces QSGW results. We discuss the trend of parameters and multiplet excitations for trivalent free rare-earth ions, and the difference in parameters of Eu ion in each material.

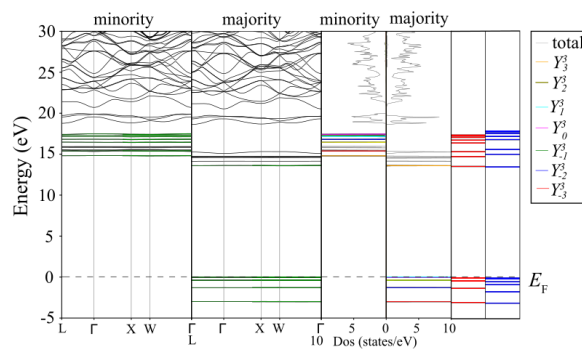


FIG. 1. (left and middle) Band structure and density of states from QSGW of free Eu ion. (right) comparison of QSGW Hamiltonian (red) and mean-field Hamiltonian (blue).

Keywords: rare-earth ion, multiplet excitation, first-principles calculation, QSGW

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TC-O02 (Oral)

Carrier-Trapping Induced Transformation of Dislocation Core Structures in Zn Compounds

Sena Hoshino^{1*}, Yu Oshima¹, Tatsuya Yokoi¹, Atsutomo Nakamura², Katsuyuki Matsunaga^{1,3}

¹ Department of Materials Physics, Nagoya University, Aichi, 464-8603, Japan

² Department of Mechanical Science and Bioengineering, Osaka University, Osaka, 560-0043, Japan

³ Nanostructures Research Laboratory, Japan Fine Ceramics Center, Aichi, 456-8587, Japan

* Corresponding author's e-mail: hoshino.sena.i9@s.mail.nagoya-u.ac.jp

Zn compound semiconductors exhibit increased deformation stress when irradiated with light [1], which is well known as the photoplastic effect (PPE). Recently, our theoretical calculations on ZnS demonstrated that Shockley partial dislocations form new like-atom bonds at the cores by trapping excess carriers [2]. Such additional bonds must be broken for dislocations to move, which is thus expected to decrease dislocation mobility. Since excess carriers are introduced by light irradiation, carrier-induced transformation of dislocation cores may be closely related to the PPE. However, it is not clear whether such phenomenon originating from dislocation cores is general in other Zn compounds. This work thus aimed to determine dislocation core structures and their energetics with and without excess carriers in ZnS, ZnSe and ZnTe.

Density-functional theory (DFT) calculations were performed using the projected augmented wave method implemented in the VASP core. The three Zn compounds examined have the zincblende structure, which typically has the easiest slip plane with {111} polar planes. In this case, two types of Shockley partial dislocation cores can be considered depending on a character of an inserted extra half plane: the Zn core and the anion core, which were modeled. Excess electrons and holes were then introduced into supercells containing the partial dislocations by changing the number of electrons.

Fig. 1 (a) shows the most stable structure for the Te core in ZnTe without excess carriers. In this case, undercoordinated Te atoms remain along the dislocation line. By contrast, the Te core transforms to a “reconstructed” structure having new Te-Te bonds in the presence of excess holes (Fig. 1(b)). The similar core transformations were also observed at the S core in ZnS [2] and Se core in ZnSe. Dislocation formation energies indicated that in the presence of excess carriers, the reconstructed dislocation cores are energetically more favorable than the unreconstructed ones, with energy differences of 0.74, 0.59 and 0.35 eV/nm in the S core, Se core and Te core, respectively. These values can be considered as the required energy to break the like-atom bonds. It is thus expected that PPE becomes more pronounced in the order of ZnS, ZnSe and ZnTe.

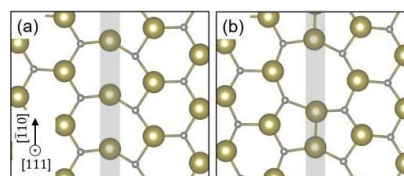


FIG. 1. Dislocation core structures for the Te core in ZnTe. Silver and golden balls indicate Zn and Te atoms, respectively. Gray lines show the dislocation lines.

Keywords: Dislocation, Carrier trapping, DFT calculation, Compound semiconductor

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