ISAMMDoF2015 Summaries

International Symposium on Advanced Materials Having Multi-Degrees-of-Freedom – Optical properties, Structural Analyses, Imaging and Informatics of Materials –

November 2-3, 2015
Kumamoto University,
Kumamoto, JAPAN

ISAMMDoF2015

2nd International Symposium on Advanced Materials Having Multi-Degrees-of-Freedom

- Optical properties, Structural analyses, Imaging and Informatics of materials -

http://phys.ipps.kumamoto-u.ac.jp/ISAMMDoF2/index.html

2nd ~ 3rd November, 2015,
Kurokami South E3 Bldg. (Faculty of Science Bldg. 3), Kumamoto University, Kumamoto JAPAN

Mon, 2nd Nov, 2015

- **Registration** — 9:00∼9:25 — 2F Lobby

- **Opening** (Prof. H. Akiyama, Director, IPPS) — 9:25∼9:30 — D201
- **Session 1** (Chair: S. Hosokawa) — 9:30∼ — D201

9:30∼10:15 **I-1**

What can we learn from table-top x-ray fluorescence holography experiments?

P. Korecki, K. M. Dabrowski, D. T. Dul

Institute of Physics, Jagiellonian University, Krakow, Poland

We discuss x-ray fluorescence holography (XFH) experiments performed using a table-top setup based on micro-focus x-ray source and polycapillary optics. By means of this setup it was possible to study some basic properties of XFH, in particular, to show the impact of matrix effects on the reconstruction of atomic structures with element sensitivity.

10:15∼11:00 **I-2**

Progress of Neutron Atomic Resolution Holography for Observations of Light Elements

K. Ohoyama[1], K. Hayashi[2], N. Happo[3], S. Hosokawa[4], M. Harada[5], Y. Inamura[5]

[1] *Ibaraki University, Japan*
[2] *Nagoya Institute of Technology, Japan*
[3] *Hiroshima City University, Japan*
[4] *Kumamoto University, Japan*
[5] *5J-PARC Center, Japan*

Present situation and progress of the atomic resolution neutron holography (NH) technique in Japan will be presented. Since neutrons are sensitive to light elements and spins in materials, NH is a quite important prove to clarify mechanisms of functionality of materials based on visualization of 3D local structures. Resent results and a future plan are also explained.

- *Coffee Break* — 11:00∼11:15 — 2F Lobby

• Session 2 (Chair: F. Shimojo) 11:15∼ D201

11:15∼12:00 **I-3**

Exploring applications of X-ray fluorescence holography

K. Hayashi

Nagoya Institute of Technology, Japan

X-ray fluorescence holography (XFH) is a method for investigating atomic order up to the medium ranges, and can provide 3D atomic images around specific elements within a radius of nanometer order. We have applied XFH to elucidation of lattice distortion in a relaxor ferroelectric and finding of nano-clusters in a high -Tc oxide ferromagnetic semiconductor. These features cannot be obtained by other methods. XFH has a great potential of exploring new field of solid state physics.

12:00∼12:45 **I-4**

3D Atomic Structure Imaging of Superconductors and Magnetic Materials by Photoelectron Holography

F. Matsui

Nara Institute of Science and Technology, Japan

We constructed an experimental end station dedicated to photoelectron diffraction measurements at BL25SU, SPring-8. The algorithm for reconstructing real space atomic arrangement images from photoelectron diffraction has been developed. Recent progress in the atomic scale structure investigations by photoelectron diffraction for carbon-based superconductor surfaces and magnetic thin films are reviewed.

○ *Lunch Break* 12:45∼13:50

• Session 3 (Chair: M. Aniya) 13:50∼ D201

13:50∼14:35 **I-5**

Chalcogenide Glasses for Phase-Change Memory: Beyond the Silicon

J. Orava

University of Cambridge, Department of Materials Science & Metallurgy, UK

Application of chalcogenide glasses in phase-change memory is discussed. The memory switching relies on reversible glassy-to-crystalline transitions in chalcogenides induced by either electrical or optical pulses. The kinetics in the supercooled liquid expressed as temperature-dependent viscosity, nucleation and crystal growth rates and related to the memory operation.

14:35∼14:50 **O-1**

Bayesian Estimation of Excitonic Absorption Spectra

K. Iwamitsu[1], S. Aihara[2], M. Okada[3,4], I. Akai[5]

[1]*Faculty of Science, Kumamoto University,*
[2]*Graduate School of Science and Technology, Kumamoto University,*
[3]*Graduate School of Frontier Sciences, The University of Tokyo,*
[4]*Brain Science Institute, RIKEN,*
[5]*Institute of Pulsed Power Science, Kumamoto University*

With the Metropolis algorithm in a Bayesian estimation, we analyzed a synthetic spectrum of excitonic absorption in Cu_2O thin films sandwiched by MgO plates. As a result, we can obtain probability distributions of all spectral parameters only using one synthetic spectrum.

14:50∼15:05 **O-2**

Bayesian deconvolution of photoluminescence spectra of yellow 1S excitons in Cu_2O thin films sandwiched by MgO plates

S. Aihara[1], K. Gunji[1], K. Iwamitsu[2], M. Okada[3,4], I. Akai[5]

[1] *Graduate School of Science and Technology, Kumamoto University,*
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We have investigated parameter estimation of synthetic data having different variance of noise, which modeled on photoluminescence spectra of yellow 1S excitons in Cu_2O thin films sandwiched by MgO plates using Bayesian statistics. We found that the parameter estimation have a limit and the distribution shapes change.

○ *Coffee Break* **15:05∼15:20** **2F Lobby**

• Short presentation for poster P-1∼P-24 **15:20∼** **D201**

• Photo **16:08∼16:15** **D201**

• Poster presentation-1 **16:15∼17:45** **D211**

P-1

Synthesis and Structure of Tetra-Acetate-Bridged Binuclear Gd(III) Complex $[(\mu_4\text{-OAc})_4(Gd^{III}H_2L)_2](ClO_4)_2$ (OAc = Acetate, H_2L = Bis(5-methylimidazol-4-yl-methylideneaminopropyl)methylamine: Toward Magnetocaloric Material

M. Ito[1], D. Hamada[1], K. Miyano[1], N. Matsumoto[1], Y. Sunatsuki[2]

[1] *Graduate School of Science and Technology, Kumamoto University,*
[2] *Department of Chemistry, Faculty of Science, Okayama University*

Tetra-acetate bridged binuclear Gd^{III} complex $[(\mu_4\text{-OAc})_4(Gd^{III}H_2L)_2(ClO_4)_2]$ was synthesized, where OAc = Acetate and H_2L = bis(5-methylimidazol-4-yl-methylideneaminopropyl)methylamine. Linear polydenate ligand H_2L functions as a bridging ligand to two Gd^{III} ions, in which the central amine is free from the coordination. Two Gd^{III} ions are bridged by four acetate groups in the classical $\eta^1 : \eta^2 : \mu_2$ fashion, and the other two bridge in the less common $\eta^2 : \eta^1 : \mu_2$ fashion. The $Gd\cdots Gd$ distance is 3.920(6) Å, that is considerably shorter than 4.183(1) Å of the bis-acetate bridged Gd^{III} complex.

P-2

Syntheses, 1D Structure via Anion-Imidazole Hydrogen Bonds, and SCO Properties of $[Fe^{III}(Him)_2$(4-MeOhapen)]Y (Y = BF_4, PF_6, AsF_6, SbF_6, CF_3SO_3)

H. Ono[1], K. Miyano[1], T. Fujinami[1], N. Matsumoto[1], Y. Sunatsuki[2]

[1] *Graduate School of Science and Technology, Kumamoto University,*
[2] *Department of Chemistry, Faculty of Science, Okayama University*

A series of iron(III) complexes, $[Fe^{III}(Him)_2$(4-MeOhapen)]Y (Y = BF_4, PF_6, AsF_6, SbF_6, CF_3SO_3), were synthesized. The anion plays as a linker to form hydrogen-bonded assembly structures of dimeric and 1D chain structures. These complexes showed several types of SCO behaviors including symmetry breaking transition.

P-3

Synthesis, Structure, Luminescence, and Magnetic Properties of Acetate-Bridged Binuclear Zinc(II)-Lanthanide(III) Complexes (Ln^{III} = Nd^{III}, Sm^{III}, Eu^{III}, Gd^{III}, Tb^{III}, Dy^{III}, Ho^{III}, Er^{III})

H. Okabe[1], N. Matsumoto[1], Y. Sunatsuki[2], M. Tsuchimoto[3]

[1] *Graduate School of Science and Technology, Kumamoto University,*
[2] *Department of Chemistry, Faculty of Science, Okayama University*
[3] *Chiba Institute of Technology*

A series of binuclear acetate-bridged zinc(II)-lanthanide(III) complexes, $[Zn^{II}(3\text{-MeOsaltn})(ac)Ln^{III}(hfac)_2]$ (Ln^{III} = Nd^{III}, Sm^{III}, Eu^{III}, Gd^{III}, Tb^{III}, Dy^{III}, Ho^{III}, Er^{III}), were synthesized and characterized. All the crystal structures have an isomorphous structure. The temperature and field dependent magnetic susceptibilities were measured and the complexes except for Zn^{II}-Gd^{III} complex showed the magnetic anisotropy.

P-4

Chiral One-dimensional Spin Crossover Iron(III) Complex with Spin Transition Temperature around Room Temperature $[Fe^{III}(Him)_2(6\text{-MeOhapacen})]BPh_4$

T. Nishida[1], K. Miyano[1], T. Fujinami[1], N. Matsumoto[1], A. Higashihara[1], R. Irie[1], Y. Sunatsuki[2]

[1] *Graduate School of Science and Technology, Kumamoto University,*
[2] *Department of Chemistry, Faculty of Science, Okayama University*

SCO Fe^{III} complex, $[Fe^{III}(Him)_2(6\text{-MeOhapacen})]BPh_4$, was synthesized and characterized. One of two imidazoles is hydrogen-bonded to the phenoxo oxygen atom of the adjacent unit to give a chiral 1D chain structure. The X-ray analyses showed significant temperature dependence of Fe-N and OFe-O dimensions, indicating a gradual spin transition around room temperature.

P-5

Tetrameric Iron(II) Complex Assembled via Imidazole $\cdots$ Chloride Hydrogen Bonds *fac*-$[Fe^{II}(HL^{n-pe})_3]Cl{\cdot}PF_6$: Structural Study of Spin Transition

M. Yamashita[1], Y. Ii[1], H. Ono[1], N. Matsumoto[1], Y. Sunatsuki[2]

[1] *Graduate School of Science and Technology, Kumamoto University,*
[2] *Department of Chemistry, Faculty of Science, Okayama University*

A spin crossover iron(II) complex, *fac*-$[Fe^{II}(HL^{n-Pen})_3]Cl{\cdot}PF_6$, was synthesized, where HL^{n-Pen} denotes 2-methylimidazol-4-yl-methylidene-*n*-pentylamine. The tetrameric cubane-like structure $\{fac\text{-}[Fe^{II}(HL^{n-Pen})_3]^{2+}\cdots Cl\}_4$ is constructed from twelve $NH\cdots Cl^-$ hydrogen bonds and this hydrogen-bonding motif gives a cubane-like structure. The magnetic data shows an abrupt one-step spin transition, which is in accord with behavior of cell volume and Fe-N distance.

P-6

Field-induced Single Ion Magnetic Properties of Mononuclear Dysprosium(III) Complex with Carbonate and Tripodal N_7 ligand $[Dy^{III}(H_3L)CO_3]Cl{\cdot}7H_2O$

A. Matsumoto[1], K. Fukushige[1], K. Sugiura[1], K. Murakami[1], N. Matsumoto[1],Y. Sunatsuki[2], M. Weselski[3], A. Bienko[3], J. Mrozinski[3]

[1] *Graduate School of Science and Technology, Kumamoto University,*
[2] *Department of Chemistry, Faculty of Science, Okayama University*
[3] *University of Wroclaw*

Mononuclear dysprosium(III) complex with CO_3^{2-} and tripod N_7 ligand, $[Dy^{III}(H_3L)CO_3]Cl{\cdot}7H_2O$, was synthesized, where H_3L = tris[2-(((imidazol-4-yl)methylidene)amino)ethyl]amine). The magnetic anisotropy and the frequency dependence of ac magnetic susceptibility under 1000 Oe are observed and the energy barrier was estimated to be Δ/k_B = 35.9 K.

P-7

Ferromagnetic Chiral One-Dimensional Polynuclear and Achiral Cyclic Tetranuclear Copper(II)-Lanthanide(III) Complexes Generated by Chiral and racemic "Ligand-Complex" Na[CuL^{dpen}]

T. Ueno[1], T. Fujinami[1], N. Matsumoto[1], M. Furusawa[1], R. Irie[1], Y. Sunatsuki[2], N. Re[3], T. Kanetomo[4], T. Ishida[4]

[1] *Graduate School of Science and Technology, Kumamoto University,*
[2] *Department of Chemistry, Faculty of Science, Okayama University*
[3] *Chieti University,*
[4] *Electro Communication University*

The 1:1 assembly reaction of racemic form of "bridging ligand-complex" $Na[Cu^{II}L^{dpen(1R2R/1S2S)}]\cdot CH_3CN$ with $Ln^{III}(NO_3)_3\cdot 6H_2O$ (Ln = Tb, Dy) in acetonitrile gives a centrosymmetric cyclic complex $[Cu^{II}L^{dpen(1R2R/1S2S)}Ln(NO_3)_2]_2$(**1Ln**) and that of enantiopure form $Na[Cu^{II}L^{dpen(1R2R)}]\cdot 2CH_3CN$ with $Ln^{II}I(NO_3)_3\cdot 6H_2O$ (Ln = Tb, Dy) in acetonitrile gives a chiral one-dimensional complex $[Cu^{II}L^{dpen(1R2R)}Ln^{III}(NO_3)_2]_\infty$(**2Ln**), respectively.

P-8

Mononuclear and Acetate-bridged One-dimensional Polynuclear Mn(III) Complexes

Y. Matsukata[1], T. Toyama[1], D. Hamada[1], N. Matsumoto[1], Y. Sunatsuki[2], N. Re[3]

[1] *Graduate School of Science and Technology, Kumamoto University,*
[2] *Department of Chemistry, Faculty of Science, Okayama University*
[3] *Chieti University,*

Mononuclear and one-dimensional polynuclear Mn^{III} complexes were synthesized and the structures were determined. Magnetic measurements of the acetate-bridged 1D complex showed a field-induced meta-magnetic transition from an antiferromagnetic state to a weak ferromagnetic phase.

P-9

Observation of Excited-state Zeeman splittings by V-type electromagnetically induced transparency in Na vapor

K. Shijo, K. Harimaya, M. Mitsunaga

Graduate School of Science and Technology, Kumamoto University,

We have observed excited-state Zeeman sublevel splitting frequencies by using V-type EIT in a sodium vapor. We used a buffer gas to suppress the SA signals and succeeded in observing V-type EIT signals. The peak positions agree quite well with theoretical predictions.

P-10

Lineshape study and ac Stark shifts in N-type resonances in Na vapor

K. Harimaya, K. Shijo, M. Mitsunaga

Graduate School of Science and Technology, Kumamoto University,

We have experimentally and theoretically demonstrated that the line shapes observed in ordinary EIT experiments in Na vapor are made up of two contributions, EIT and NTR. And, we have also studied ac Stark shifts for EIT and NTR; it was found that, for NTR, the shift can be nullified.

P-11

Photoluminescence spectra in Cu_2O thin crystals and their polarization dependences

K. Gunji[1], S. Aihara[1], F. Ichikawa[1], I. Akai[2]

[1] *Graduate School of Science and Technology, Kumamoto University,*
[2] *Institute of Pulsed Power Science, Kumamoto University*

We have studied polarization dependences of photoluminescence (PL) spectra in Cu_2O thin crystals sandwiched by MgO plates. In such crystals, the 1S ortho excitons split into two and three levels. We found that the PL intensities of the excitons show different polarization dependences and discussed these dependences.

P-12

Optimal Growth Condition of Layered Semiconductor BiI_3 Grown by Hot-Wall Method

R. Sakamoto[1], K. Iwamitsu[2], S. Aihara[1], F. Ichikawa[2], T. Shimamoto[3], I. Akai[3]

[1] *Graduate School of Science and Technology, Kumamoto University,*
[2] *Faculty of Science, Kumamoto University*
[3] *Institute of Pulsed Power Science, Kumamoto University*

We studied the growth condition of BiI_3 thin films grown by hot-wall method. It is found that the α-Al_2O_3(0001) is the best substrate and the evaporation rate of ~ 1.0 Å/s is the optimal growth condition.

P-13

Long continuing coherent phonon in a bismuth thin-film

M. Hamamoto[1], K. Iwamitsu[2], I. Akai[3]

[1] *Graduate School of Science and Technology, Kumamoto University,*
[2] *Faculty of Science, Kumamoto University*
[3] *Institute of Pulsed Power Science, Kumamoto University*

We have investigated the long continuing coherent phonon (CP) in a bismuth thin film. It is found that the CP signal could be modeled by a damped oscillator and its Fourier spectrum only have an A_{1g} mode peak.

• Poster presentation-2

16:15∼17:45 D314

P-14

Polarization of Photoluminescence of $Cd_{0.8}Mn_{0.2}Te$ under High Density Excitation of Localized Excitons

M. Nagata, T. Hirase, K. Miyajima

Department of Applied Physics, Graduate School of Science, Tokyo University of Science

The generation of spin-aligned high-density exciton magnetic polarons (HD-EMPs) was reported for $Cd_{0.8}Mn_{0.2}Te$. We found the two mechanisms of spin alignment of HD-EMPs. One follows the spins of photoexcited carriers, and other is a spontaneous spin-alignment along a certain axis resulting from the interaction with Mn ions.

P-15

Crystallinity of tin oxide films grown by mist-CVD at atmospheric pressure

J. Matsushita[1], T. Otabe[1], T. Abe[1], K. Sue[2], Y. Nakamura[1,2]

[1] *Graduate School of Science and Technology, Kumamoto University,*
[2] *Faculty of Engineering, Kumamoto University,*
[3] *Kumamoto Institute for Photo-Electro Organics*

To develop new materials for light emitting diodes, we have investigated SnO_2 as a host material. SnO_2 films have been formed on m-plane (10-10) sapphire substrates by mist chemical vapor deposition at atmospheric pressure. The samples were characterized by X-ray diffraction, and SnO_2 films were found to be epitaxially grown on sapphire substrates.

P-16

Ion implantation of Phosphorus into ZnO films formed by mist-CVD

Y. Yokoyama[1], S. Wada[1], J. Oshino[1], Y. Naka[1], S. Nagaoka[2,3], Y. Nakamura[1,3]

[1] *Graduate School of Science and Technology, Kumamoto University,*
[2] *Kumamoto Industrial Research Institute,*
[3] *Kumamoto Institute for Photo-Electro Organics*

Formation of p-type ZnO is inevitable to develop ZnO-based light emitting diodes. In this study, we have formed P-doped ZnO by ion implantation of P and subsequent annealing for the ZnO layer epitaxially grown by mist chemical vapor deposition. The samples were characterized by several measuring methods, and we discuss the mechanism.

P-17

A Crystallochemical Approach to Chalcogenide Glasses

Y. Harada, M. Aniya

Graduate School of Science and Technology, Kumamoto University,

The properties of chalcogenide glasses are analyzed from a crystallochemical point of view. The similarity between phase change materials and ion conducting chalcogenide glasses is pointed out. The relation between the activation energy of ion transport and the optical band gap supports the bond fluctuation model of superionic conductors.

P-18

The Grüneisen Parameter of Ionic Conductors

E. Hirano, M. Aniya

Graduate School of Science and Technology, Kumamoto University,

The Gruneisen parameter is a quantity that reflects the anharmonicity of lattice vibration. The temperature dependence of this quantity is weak in most materials. However, in ionic conductors we have found anomalously large temperature dependence of this quantity.

P-19

Configuration Entropy of Polymer Electrolytes: Evaluation based on the Bond Strength-Coordination Number Fluctuation Model

T. Morishita[1], E. Hirano, [1] M. Ikeda[2],M. Aniya[1]

[1] *Graduate School of Science and Technology, Kumamoto University,*
[2] *National Institute of Technology, Fukui College*

The Bond Strength-Coordination Number Fluctuation (BSCNF) model has been proposed originally to describe the temperature dependence of the viscosity of supercooled liquids. In the present study, the configuration entropy in polymer electrolytes is evaluated using an expression derived based on the BSCNF model.

P-20

A Model for the Particle Size Dependence of the Ionic Conductivity

K. Hagihara, M. Aniya

Graduate School of Science and Technology, Kumamoto University,

The particle size dependence of the ionic conductivity is calculated based on the Brick-Layer Model. The result indicates that the ionic conductivity increases by decreasing the particle size up to 100 nm, and decreases below that size.

P-21

A Theoretical Model for the Non-Arrhenius Ionic Conductivity in Solid Electrolytes

Y. Okada[1], M. Ikeda[2], M. Aniya[1]

[1] *Graduate School of Science and Technology, Kumamoto University,*
[2] *National Institute of Technology, Fukui College*

A model for the non-Arrhenius ionic conductivity of solid electrolytes is developed by applying the formulation of the Bond Strength-Coordination Number Fluctuation model. Various types of solid electrolyte are analyzed by the model and the results are related to the nature of the chemical bond.

P-22

Static Structure of V_2O_5 Glass : *Ab Initio* Molecular Dynamics Simulations

Y. Kodama, A. Koura, F. Shimojo, S. Hosokawa

Department of Physics, Kumamoto University

We performed *ab initio* molecular dynamics simulation to investigate the structure and the electronic state of V_2O_5 glass. We found that 90 % of V atoms form VO_4 unit, and the rest form VO_5 units. Two types of V-O bonds are formed depending on the coordination number of O atoms.

P-23

Photocarrier Recombination Dynamics in Halide Organometal Perovskite: Nonadiabatic *Ab initio* Molecular Dynamics simulations

T. Hakamata[1], K. Shimamura[1,2], F. Shimojo[1], R. K. Kalia[3], A. Nakano[3], P. Vashishta[3]

[1] *Department of Physics, Kumamoto University,*
[2] *Graduate School of System Informatics, Kobe University,*
[3] *Collaboratory for Advanced Computing and Simulations, University of Southern California*

We perform nonadiabatic *ab initio* molecular dynamics simulations to elucidate the mechanisms of photocarriers transport and to investigate the function methylammonium molecules. We confirm that free charge carriers are generated, and that the rotation of methylammonium molecules is associated with the charge separation.

P-24

XAFS analysis of $TlInSe_2$ thermoelectric material

K. Kamimura[1], S. Hosokawa[1], N. Happo[2], K. Mimura[3], N. Mamedov[4]

[1] *Kumamoto University, Japan,*
[2] *Hiroshima City University, Japan,*
[3] *Osaka Prefecture University, Japan,*
[4] *Azerbaijan National Academy of Sciences, Azerbaijan*

The local structure around the Tl atoms in $TlInSe_2$ thermoelectric material was investigated by XAFS measurements. The Tl-Tl interatomic distance obtained from XAFS is much smaller than that obtained from x-ray diffraction at room temperature, which suggests a formation of the dimerization Tl atoms on the chain direction.

P-25

Local structure of Fe-Ni Inver alloy studied by x-ray fluorescence holography

S. Hosokawa[1], Y. Ideguchi[1], K. Kamimura[1], K. Kimura[1], N. Happo[2], K. Hayashi[3]

[1] *Kumamoto University, Japan,*
[2] *Hiroshima City University, Japan,*
[3] *Nagoya Institute of Technology, Japan*

Fe and Ni $K\alpha$ x-ray fluorescence holography measurements were performed on a $Fe_{66}Ni_{34}$ Invar alloy. The atomic images around Ni show a *fcc* structure, while those around Fe exhibit a *bcc*-like arrangement. This result suggests that the Invar effect would be explained by a gradual structural change from sparse *bcc* to dense *fcc*.

• Casual reception **18:00∼** **Forico**

Tue, 3rd Nov, 2015

• Session 4 (Chair: Y. Nakamura) 9:00∼ D201

9:00∼9:45 **I-6**

ZnO: From Optoelectronic Materials to Devices

C. X. Shan, B. H. Li, S. P. Wang, M. M. Jiang, D. Z. Shen

State Key Laboratory of Luminescence and Applications, Changchun Institute of Optics, Fine Mechanics and Physics, Chinese Academy of Sciences, China

p-type ZnO films have been realized by employing lithium-nitrogen codoping method, and LEDs and ultraviolet photodetectors have been fabricated from the p-ZnO. The LEDs can work continuously for 97 hours, and the photodetectors can still work after five months, indicating the acceptable reliability of the devices.

9:45∼10:30 **I-7**

Optical Polarization Properties and Carrier Recombination Dynamics in InGaN Quantum Wells

A. A. Yamaguchi

Optoelectronic Device System Research & Development Center, Kanazawa Institute of Technology, Japan

InGaN-based optical devices such as blue/green/white LEDs and blue-violet laser diodes, have been widely used. However, high-performance optical devices have been realized within limited wavelength region compared with their potential bandgap coverage. In this paper, material issues of the InGaN optical devices from the viewpoint of optical characterizations are discussed.

10:30∼11:00 **I-8**

Doping Effect on Photoabsorption and Charge Dynamics in Molecular Graphene-Fulleren Heterojunction

S. Ohmura[1], K. Tsuruta[2], F. Shimojo[3], A. Nakano[4]

[1] *Research Center for Condensed Matter Physics, Hiroshima Institute of Technology,*
[2] *Department of Electrical and Electronic Engineering, Okayama University,*
[3] *Department of Physics, Kumamoto University,*
[4] *Collaboratory for Advanced Computing and Simulation, University of Southern California*

Doping effect on optical response of a molecular graphene (HBC) with covalently linked fullerene, a building block in a self-assembled supramolecular solar cell, has been explored by using ab-initio theoretical methods. We have investigate light absorption spectra and charge dynamics of the molecule with doped HBC.

○ *Coffee Break* 11:00∼11:15 2F Lobby

• Session 5 (Chair: D. Kosumi) 11:15∼ D201

11:15∼11:45 **I-9**

Quantum beats of quantum confined exciton states in quantum wells

A. V. Trifonov

Spin Optics Laboratory, Saint-Petersburg State University, Russian Federation

Quantum beats of a system of the coherently excited quantum confined exciton states in a high-quality InGaAs/GaAs quantum well are experimentally detected. The beat signal is observed both at positive and at negative delays. Several QB frequencies are, which coincide with the interlevel spacings in the exciton system.

11:45∼12:00 **O-3**

Syntheses, Structure, and Magnetic Properties of Carbonate-Bridged $Ni^{II}_2Ln^{III}_2$ Complexes (Ln^{III}= Gd^{III}, Tb^{III}, Dy^{III}) Generated by Atmospheric CO_2 Fixation

D. Hamada[1], S. Sakamoto[1], T. Fujinami[1], N. Matsumoto[1], Y. Sunatsuki[2]

[1] *Graduate School of Science and Technology, Kumamoto University,*
[2] *Department of Chemistry, Faculty of Science, Okayama University*

Atmospheric CO_2 fixation occurred in a basic reaction condition gave the three series of $Ni^{II}_2Ln^{III}_2$ complexes, crystallized into an isomorphous structure. The temperature-dependent magnetic susceptibilities indicated a ferromagnetic interaction between Ni^{II} and Ln^{III} for all the complexes, with a distinct different magnetic behavior in the lowest between Ln^{III} and Ln^{III}.

12:00∼12:15 **O-4**

Spin Transition between High-spin (HS) and an Ordered Symmetry Breaking (3HS-LS) States of Fe^{III} Complex $[Fe^{III}(Him)_2(4\text{-}MeOhapen)]CF_3SO_3$

K. Miyano[1], T. Nishida[1], H. Ono[1], D. Hamada[1], T. Fujinami[1], N. Matsumoto[1], Y. Sunatsuki[2]

[1] *Graduate School of Science and Technology, Kumamoto University,*
[2] *Department of Chemistry, Faculty of Science, Okayama University*

The unequal population of the HS and LS states of [HS(D)-HS(C)-HS(B)-LS(A)] is the result of molecular shrinkage and geometrical change of A, the conformational change of the saturated five-membered chelate ring of C, and a rearrangement of hydrogen bond network within a framework of 1D structure. The present result suggests that multi-step spin transition with all the spin states can be observed for this type of one-dimensional complexes.

○ *Lunch Break* **12:15∼13:30**

• Session 6 (Chair: S. Ohmura) **13:30∼** **D201**

13:30∼14:15 **I-10**

Conformational analysis of long-chain cyclodextrin for drug delivery application

M. Kunaseth

Nanoscale Simulation Laboratory, National Nanotechnology Center (NANOTEC), National Science and Technology Development Agency (NSTDA), Thailand

We proposed the new structural parameters to study large-ring cyclodextrins (CD14) conformations, which were used to properly identify CD14 conformations for inclusibility of drug molecule via "openness" of the ring. Population analysis based on these parameters was also presented.

14:15∼14:45 **I-11**

Non-Arrhenius transport property in glass-forming materials

M. Ikeda[1], M. Aniya[2]

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The non-Arrhenius (NA) temperature dependence of the transport coefficients is often described by the Vogel-Fulcher-Tammann (VFT) equation. In our recent study, it was shown that the VFT-like patterns can be described by the bond strength-coordination number fluctuation (BSCNF) model. In the present study, the NA transport property is discussed based on the BSCNF model.

14:45∼15:00 **O-5**

Static structure of glass $Ag_x(GeSe_3)_{1-x}$ based on *ab initio* molecular dynamics study

A. Koura, F. Shimojo, S. Hosokawa

Department of Physics, Kumamoto University

We have investigated the static structure of glass $Ag_x(GeSe_3)_{1-x}$ (x = 0.15, 0.3 and 0.50) based on *ab initio* molecular dynamics simulations. Even at the the lower concentration $x = 0.15$, Ag-Ag homopolar covalent bonds sometimes appear and short chain chain-type fragments type are formed.

15:00∼15:15 **O-6**

Orientation Dependence of Shock Wave Propagation in Molecular Crystals: *Ab Initio* **Molecular Dynamics Simulations**

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We perform *ab initio* molecular dynamics simulations combined multiscale shock technique to elucidate the orientation dependence of chemical reactions associated with shock wave propagation in van der Waals crystal. It is clarified that shock normal to multilayers becomes more sensitive, producing water molecule assisted by inter-layer nitrogen-nitrogen bond formation.

• Closing (I. Akai) **15:15∼15:20** **D201**