LIST OF POSTER PRESENTATIONS

December 10, 2010 Fri. 19:00-21:00

- PS-1 Terahertz emission from GaAs films on Si(100) and Si(111) substrates grown by molecular beam epitaxy <u>Takashi Yoshioka</u>, Elmer Estacio, Satoru Takatori, Pham Hong Minh, Marilou Cadatal-Raduban, Tomoharu Nakazato, Toshihiko Shimizu, Nobuhiko Sarukura, John Vincent Misa, Rafael Jaculbia, Michael Defensor, Armando Somintac, and Arnel Salvador Institute of Laser Engineering, Osaka University, Yamadaoka, Suita, Osaka, Japan
- PS-2 A first-principles study on water flow through single-walled carbon nanotubes with the aid of artificial neural network and statistical methods <u>Samad Ahadian</u>, Hiroshi Mizuseki, Yoshiyuki Kawazoe Institute for Materials Research (IMR), Tohoku University, Sendai, Japan
- PS-3 Effect of chirality on the π-π stacking interaction of Guanine with SWCNT <u>M. Rajarajeswari</u>, K. Iyakutti, and Y. Kawazoe School of Physics, Madurai Kamaraj University, Madurai, Tamil Nadu, India
- PS-4 Role of electric field on desorption of chemisorbed hydrogen from carbon nanostructures, SWCNT and C₆₀
 <u>V. J. Surya</u>, K. Iyakutti, H. Mizuseki and Y. Kawazoe
 School of Physics, Madurai Kamaraj University, Madurai, Tamil Nadu, India
- PS-5 A genetic algorithm for designing binary atomic cluster
 <u>Akito Taneda</u> and Yoshiyuki Kawazoe
 Graduate School of Science and Technology, Hirosaki University, Aomori, Japan
- PS-6 Ab-initio study of opto-electronic properties of IAO and IATO
 <u>Madhvendra Nath Tripathi</u>, R. Sahara, H. Mizuseki, and Y. Kawazoe
 Institute for Materials Research (IMR), Tohoku University, Sendai, Japan
- PS-7 Fabrication and characterization of Cu₂O-based solar cells
 <u>Kazuya Fujimoto</u>, Takeo Oku, Tsuyoshi Akiyama, Atsushi Suzuki
 Department of Materials Science, The University of Shiga Prefecture, Shiga, Japan
- PS-8 Fabrication and characterization of organic solar cells using polythiophene films by electrochemical polymerization Koji Goto, Tsuyoshi Akiyama, Takeo Oku, Atsushi Suzuki
 Department of Materials Science, The University of Shiga Prefecture, Shiga, Japan
- PS-9 Fabrication of polyaniline thin films by electropolymerization and its application for organic solar cells Kei Inoue, Atsushi Suzuki, Tsuyoshi Akiyama and Takeo Oku Department of Materials Science, The University of Shiga Prefecture, Shiga, Japan

- PS-10 Effects of Au nanoparticles addition to hole transfer layer in organic solar cells based on copper naphthalocyanine and fullerene
 <u>Akihiko Nagata</u>, Takeo Oku, Tsuyoshi Akiyama, Atsushi Suzuki
 Department of Materials Science, The University of Shiga Prefecture, Shiga, Japan
- PS-11 Fabrication and characterization of tetracyanoquinodimethane-based solar cells Takahiro Ohtsuki, <u>Atsushi Suzuki</u>, Takeo Oku, Tsuyoshi Akiyama Department of Materials Science, The University of Shiga Prefecture, Shiga, Japan
- PS-12 Effects of chiral index on magnetic properties of N@C₆₀, C₅₉N and (N@C₆₀)₂ within single-walled carbon nanotube as peapods
 <u>Atsushi Suzuki</u>, Takeo Oku
 Department of Materials Science, The University of Shiga Prefecture, Shiga, Japan
- PS-13 Formation and characterization of phthalocyanine dimer solar cells
 <u>Akihiro Takeda</u>, Takeo Oku, Atsushi Suzuki, Tsuyoshi Akiyama, Yasuhiro Yamasaki
 Department of Materials Science, The University of Shiga Prefecture, Shiga, Japan
- PS-14 Study on silicon-based organic/inorganic solar cells
 Kazumi Yoshida, Takeo Oku, <u>Tsuyoshi Akiyama</u>, Atsushi Suzuki Youichi Kanamori, and Mikio Murazono
 Department of Materials Science, The University of Shiga Prefecture, Shiga, Japan
- PS-15 Microstructures and properties of spherical silicon solar cells with anti-reflection layers Tatsuya Yoshikawa, <u>Tsuyoshi Akiyama</u>, Takeo Oku, Satoru Seo, Yoshimasa Ohnishi, Katsumi Yagi, Mikio Murozono
 Department of Materials Science, The University of Shiga Prefecture, Shiga, Japan
- PS-16 Spill over kinetics of H₂ molecule on Al (111) surface
 <u>Qi Peng</u>, Hiroshi Mizuseki, and Yoshiyuki Kawazoe
 Institute for Materials Research, Tohoku University, Sendai, Japan
- PS-17 Evaluation of Ce:LLF as scintillator by using SRFEL
 <u>Tomoharu Nakazato</u>, Yusuke Furukawa, Marilou Cadatal-Raduban, Minh Pham, Toshihiro Tatsumi,
 Ayumi Saiki, Yasunobu Arikawa, Nobuhiko Sarukura, Hiroaki Nishimura, Hiroshi Azechi, Kunioki Mima,
 Tsuguo Fukuda, Masahito Hosaka, Masahiro Katoh, and Nobuhiro Kosugi
 Institute of Laser Engineering, Osaka University, Suita, Osaka, Japan
- PS-18 Equilibration of long chain polymer melts by MD/Continuum hybrid method <u>Y. Senda</u>, J. Blomqvist and R. M Nieminen Department of Applied Science, Yamaguchi University, Yamaguchi-Ube, Japan
- PS-19 Elastic and Inelastic Current through Benzene: A Self-consistently Study
 <u>Y.Y. Liang</u>, H. Chen, H. Mizuseki, Y. Kawazoe
 Institute for Materials Research, Tohoku University, Sendai, Japan

- PS-20 CO and H₂S Adsorption on Clean and Alkali-promoted Fe (100) Surface: A Density Functional Theory Study <u>Muhammad Haris Mahyuddin</u>, Rodion V. Belosludov, Hiroshi Mizuseki, Yoshiyuki Kawazoe Institute for Materials Research, Tohoku University, Sendai, Japan
- PS-21 Fast-response ZnO scintillator for evaluation of timing between X-ray free-electron laser and conventional laser Kohei Yamanoi, Kohei Sakai, Marilou Cadatal-Raduban, Tomoharu Nakazato, Toshihiko Shimizu, Nobuhiko Sarukura, Masataka Kano, Akira Wakamiya, Dirk Ehrentraut, Tsuguo Fukuda, Mitsuru Nagasono, Tadashi Togashi, Shinichi Matsubara, Kensuke Tono, Atsushi Higashiya, Makina Yabashi, Hiroaki Kimura, Haruhiko Ohashi, and Tetsuya Ishikawa Institute of Laser Engineering, Osaka University, Osaka, Japan
- PS-22 Evaluation of two-photon absorption in polystyrene-derivative material for laser-induced inertial-confinement fusion Kozue Watanabe, Yuki Minami, Kohei Yamanoi, Yasunobu Arikawa, Yumi Kaneyasu, Yumiko Suzuki, Shinji Machi, Marilou Cadatal-Raduban, Toshihiko Shimizu, Hirofumi Homma, Nobuhiko Sarukura, Mitsuo Nakai, Takayoshi Norimatsu, Hiroshi Azechi Institute of Laser Engineering, Osaka University, Osaka, Japan
- PS-23 Nd³⁺-doped fluoride crystals as vacuum ultraviolet laser materials <u>Marilou Cadatal-Raduban</u>, Kohei Yamanoi, Toshihiko Shimizu, Masahiro Kouno, Mizuki Tsuboi, Yusuke Furukawa, Minh Pham, Tomoharu Nakazato, Nobuhiko Sarukura, Toshihisa Suyama, Kentaro Fukuda, Akira Yoshikawa, and Fumio Saito Institute of Laser Engineering, Osaka University, Osaka, Japan
- PS-24 Multi-Pumped Laser Amplification Using Micro-Pulling Down Method-Grown Ce:LiCAF Crystal Masahiro Kouno, Jacque Lynn Gabayno, Marilou Cadatal-Raduban, Minh Pham, Kohei Yamanoi, Elmer Estacio, Wilson Garcia, Tomoharu Nakazato, Toshihiko Shimizu, Nobuhiko Sarukura, Toshihisa Suyama, Kentaro Fukuda, Kyoung Jin Kim, Akira Yoshikawa, and Fumio Saito Institute of Laser Engineering, Osaka University, Osaka, Japan
- PS-25 Theoretical investigation of non-stoichiometry and related point defects in Langatate piezoelectric crystal <u>Chan-Yeup Chung</u>, Ritsuko Yaokawa, Hiroshi Mizuseki and Yoshiyuki Kawazoe Institute for Materials Research, Tohoku University, Sendai, Japan
- PS-26 Single Molecule Conductance of Perfluorinated Bipyridyl Ethynes: Mechanism of Molecule-Electrode Binding <u>L. J. Kang</u>, Y. Y. Liang, H. Mizuseki, and Y. Kawazoe Institute for Materials Research, Tohoku University, Sendai, Japan
- PS-27 Atomistic Simulation of The Early Stage of Si (001) Dry Oxidation <u>Mauludi Ariesto Pamungkas</u>, Minwoong Joe, Byung-Hyun Kim, Gyubong Kim, Kwang-Ryeol Lee Computational Science Center, Korea Institute of Science and Technology, Seoul, Korea
- PS-28 Optimization of direct drive inertial confinement fusion for the National Ignition Facility <u>Mizuki Tsuboi</u>, Nobuhiko Sarukura, Masakatsu Murakami Institute of Laser Engineering, Osaka University, Osaka, Japan

- PS-29 Molecular dynamics simulations of imprint behaviors in ferroelectric thin-film capacitors <u>T. Nishimatsu</u>, Y. Kawazoe, U. V. Waghmare Institute for Materials Research (IMR), Tohoku University, Sendai, Japan
- PS-30 A simple rubber model cross-linked with ideal chains <u>Yuto Toriumi</u> and Kaoru Ohno Department of Physics, Yokohama National University, Yokohama Japan
- PS-31 The Jahn-Teller Effect and Peculiar Magnetic Interactions in AlN:Cr <u>Takeshi Fujita</u> and Hannes Raebiger Department of Physics, Yokohama National University, Yokohama Japan
- PS-32 Second-order and GW corrections to Hartree-Fock approximation for atoms: All-electron mixed basis approach <u>Yoichi Tadokoro</u>, Soh Ishii, Yoshifumi Noguchi, and Kaoru Ohno Department of Physics, Graduate School of Engineering, Yokohama National University, Yokohama, Japan
- PS-33 The relationship of physical and model charges for transition metal atoms in the different coordination octahedral cobalt complexes
 <u>S. Fukutomi</u> and H. Raebiger
 Department of Physics, Yokohama National University, Yokohama, Japan
- PS-34 STRUCTURAL INFORMATION ON C₃H₈ GAS HYDRATE FROM QUASI-HARMONIC LATTICE DYNAMICS
 <u>Maaouia Souissi</u>, Rodion V. Belosludov, Hiroshi Mizuseki, Yoshiyuki Kawazoe, Oleg S. Subbotin and Vladimir R. Belosludov
 Institute for Materials Research (IMR), Tohoku University, Sendai, Japan
- PS-35 High-pressure phases of hydrogen cyanide <u>Mohammad Khazaei</u>, Mohammad Saeed Bahramy, Fabio Pichierri, Keivan Esfarjani, and Yoshiyuki Kawazoe Institute for Materials Research (IMR), Tohoku University, Sendai, Japan
- PS-36 Electronic states of metallic peanut-shaped fullerene polymers
 <u>Yusuke Noda</u> and Kaoru Ohno
 Department of Physics, Yokohama National University, Yokohama, Kanagawa, Japan
- PS-37 Molecular dynamics simulation study of silicon nanowires oxidation <u>Byung-Hyun Kim</u>, Mina Park, Mauludi Ariesto Pamungkas, Kwang-Ryeol Lee, and Yong-Chae Chung Computational Science Center, Interdisciplinary Fusion Technology Division, KIST, Seoul, Korea
- PS-38 Understanding Ar ion induced structural modification of polymers surface and its dependency on ion energy and polymer backbones (PE and PDMS): Molecular Dynamics and experiments <u>Chansoo Kim</u>, Sk. Faruque Ahmed, Myoung-Woon Moon, Kwang-Ryeol Lee Computational Science Center, Korea Institute of Science and Technology (KIST), Korea

- PS-39 Theoretical Study on Grain Boundaries in Multicrystalline Silicon <u>Hiroshi Mizuseki</u>, Ambigapathy Suvitha, Ryoji Sahara and Yoshiyuki Kawazoe Institute for Materials Research (IMR), Tohoku University, Sendai, Japan
- PS-40 Controlling 3D Percolation by Modulating the Granular Size of Materials <u>K. Shida</u>, R. Sahara, M.N. Tripathi, H. Mizuseki, and Y. Kawazoe Institute for Materials Research (IMR), Tohoku University, Sendai, Japan
- PS-41 Investigation of magnetism in graphene nanoribbons and graphene molecules by first-principle calculations <u>N. Gorjizadeh</u>, Norio Ota, Y. Kawazoe Institute for Materials Research (IMR), Tohoku University, Sendai, Japan
- PS-42 Development of the apparatus for cryogenic cooling of metal cluster ions by He droplets -Incorporation of cobalt ions into rare gas clusters <u>Hideho Odaka</u>, Masahiko Ichihashi
 Genesis Research Institute, Inc., Ichikawa, Chiba, Japan
- PS-43 Absorption and desorption behavior of CO₂ on doped CaO surface
 <u>S. Sasaki</u>, S. Ueda, R. Inoue, R. Belosludov, Y. Kawazoe, and T. Ariyama
 Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai, Japan
- PS-44 Incorporation of surface correction and anharmonic correction to vacancy formation energy for nickel and copper: bridging the gap between Density Functional Theory and experiment
 <u>Prithwish Kumar Nandi</u> and M. C. Valsakumar
 Materials Science Group, Indira Gandhi Centre for Atomic Research, Kalpakkam, Tamil Nadu, India
- PS-45 Theoretical Study of Host-guest Interaction in Metal-Organic Framework Materials <u>R. V. Belosludov</u>, H. Mizuseki, and Y. Kawazoe Institute for Materials Research (IMR), Tohoku University, Sendai, Japan
- PS-46 Infrared spectroscopic study of the reaction mechanism of one-dimensional metallic peanut-shaped C₆₀ polymer
 <u>A. Takashima</u>, M. Nishiyama, and J. Onoe
 Department of Nuclear Engineering, Tokyo Institute of Technology, Japan
- PS-47 Chemical engineering of adamantane by lithium: A promising candidate for hydrogen storage <u>Ahmad Ranjbar</u>, Mohammad Khazaei, Natarajan Sathiyamoorthy Venkataramanan, Hoonkyung Lee, and Yoshiyuki Kawazoe Institute for Materials Research (IMR), Tohoku University, Sendai, Japan
- PS-48 Theoretical study on GFT-based first principles molecular dynamics and hydrogen quantum effect <u>Tomomi Shimazaki</u> and Momoji Kubo Graduate School of Engineering, Tohoku University, Sendai, Japan

- PS-49 Sintering Processes of Ni/YSZ Nanoparticle in Solid Oxide Fuel Cell: A Study by Molecular Dynamics Simulation <u>Jingxiang Xu</u>, Ryota Sakanoi, Takeo Matsuyama, Miho Nakamura, Nobuki Ozawa, Tomomi Shimazaki, Momoji Kubo Fracture and Reliability Research Institute, Graduate School of Engineering, Tohoku University, Sendai, Japan
- PS-50 First-principles prediction of half-metallic ferromagnetic in Mn doped β phase Ge₃N₄
 <u>V. Wang</u>, W. Xiao, E. H. Zhang, S. L. Zhang, W. T. Geng and Y. Kawazoe
 Department of Applied Physics, Xi'an Jiaotong University, Xi'an, China
- PS-51 Development of Aluminum Hydrogen Storage Material <u>Masahiko Katagiri</u> National Institute for Materials Science, Tsukuba, Ibaraki, Japan
- PS-52 Development of Raman intensity calculation code in first-principles all-electron LCAO program, DMol³ <u>Tsuguo Morisato</u> Accelrys K.K., Tokyo, Japan
- PS-53 Role of hydrogen on early stage stress corrosion cracking initiation process: A computational chemistry approach <u>Nishith Kumar Das</u> and Tetsuo Shoji Fracture and Reliability Research Institute & New Industry Creation Hatchery Center, Tohoku University, Sendai, Japan
- PS-54 Reactant promoted oxygen dissociation on gold clusters <u>Andrey Lyalin</u> and Tetsuya Taketsugu Division of Chemistry, Graduate School of Science, Hokkaido University, Sapporo, Japan
- PS-55 Adsorption of Au and Au₂ on h-BN Surface
 Min Gao, <u>Andrey Lyalin</u> and Tetsuya Taketsugu
 Division of Chemistry, Graduate School of Science, Hokkaido University, Sapporo, Japan