LIST OF POSTER PRESENTATIONS

November 23, 2012 Fri. 17:30-20:00

| PS-1 | Spatial Resolution Measurement of Hydrothermal Method Grown ZnO Crystal as a Soft X-ray Scintillator |
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| | Tomoharu Nakazato, Toshihiko Shimizu, Kohei Yamanoi, Kohei Sakai, Kohei Takeda, Ryosuke Nishi, |
| | Yuki Minami, Marilou Cadatal-Raduban, Nobuhiko Sarukura, Hiroaki Nishimura, Hiroshi Azechi, |
| | Tsuguo Fukuda, Momoko Tanaka, Masaharu Nishikino and Tetsuya Kawachi |
| | Institute of Laser Engineering, Osaka University, Osaka, Japan |

PS-2 Simulation of Structures and Phase Transitions for Helium Hydrates
Based on Ice I_h and Ice II at Low Temperatures and high pressures
Yu. Yu. Bozhko, O.S. Subbotin, R.V. Belosludov, H. Mizuseki, Y. Kawazoe, V.R. Belosludov and V.M. Fomin
Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia

PS-3 Theoretical Study of the Collective Vibration Features in Amorphous Ices

K.V. Gets, O. S. Subbotin, V. R. Belosludov, R.V. Belosludov, H. Mizuseki and Y. Kawazoe

Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia

PS-4 Thermodynamic Investigations of the Structures and Composition of

Multicomponent Hydrates (N₂-O₂-CH₄-H₂O)

<u>T.P. Adamova</u>, O.S. Subbotin, V.R. Belosludov, R.V. Belosludov, H. Mizuseki and Y. Kawazoe

Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia

PS-5 H₂-Ar Clathrate Hydrates as a Hydrogen Storage Material Ravil Zhdanov, Oleg Subbotin, Vladimir Belosludov, Rodion Belosludov, Hiroshi Mizuseki and Yoshiyuki Kawazoe Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia

PS-6 Prediction of Mechanical Behavior with Image-Based Finite Element Analysis for Periodic Microstructure

<u>Sujit Bidhar</u>, Ikumu Watanabe

National Institute of Material Science, Ibaraki, Japan

PS-7 Half-Life of ⁷Be Atom Encapsulated in Carbon Nanotubes: A First-Principles Study

<u>Shota Ono</u>, Riichi Kuwahara and Kaoru Ohno

Department of Physics, Graduate School of Engineering, Yokohama National University, Kanagawa, Japan

PS-8 Temperature and Pressure Dependent Geometry Optimization and Elastic Constant
Calculations for Arbitrary Symmetry Crystals: Applications to MgSiO₃ Perovskites
Bin Wen, Tianjiao Shao, Roderick Melnik, Yoshiyuki Kawazoe and Yongjun Tiana
State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, Qinhuangdao, China

PS-9 *Ab inito* Study of Tuning Calixarenes for the Selective Sorption of Toxic Gases

N.S. Venkataramanan, H. Mizuskei and Y. Kawazoe

Institute for Materials Research, Tohoku University, Miyagi, Japan

PS-10 DFT Calculations of H Impurity in ZnO Crystals

A.B. Usseinov, T.M. Inerbaev and A.T. Akilbekov

Physical and Technical Department, Gumilyov Eurasian National University, Astana, Kazakhstan

PS-11 Influence of Ionization Radiation on Defect Structure of LiF Crystals

R. Kassymkanova, T. Inerbaev and A.K. Dauletbekova

Physical and Technical Department, Gumilyov Eurasian National University, Astana, Kazakhstan

PS-12 Multicomponent Molecular Orbital Study on Positron Attachment to

Atoms and Molecules Based on the Virial Theorem

Takayuki Oyamada and Masanori Tachikawa

Yokohama City University, Kanagawa, Japan

PS-13 VUV Fluorescence from Nd³⁺:LuLiF₄ Excited by FEL, F₂ Laser and Third Harmonic Ti:Sapphire Laser

Ren Arita, Tatsuhiro Hori, Kohei Yamanoia, Yuki Minami, Ryosuke Nishi, Yuki Shinzato,

Mizuki Tsuboi, Mui Viet Luong, Tomoharu Nakazato, Toshihiko Shimizu, Nobuhiko Sarukura,

Marilou Cadatal-Raduban, Minh Hong Pham, Hung Dai Nguyen, Yuui Yokota, Akira Yoshikawa,

Mitsuru Nagasono and Tetsuya Ishikawa

Sustainable Energy and Environmental Engineering, Osaka University, Osaka, Japan

PS-14 Pump and Probe Experiment of ZnO Using Free Electron Laser and Synchronously-Operated Femtosecond Laser

Tatsuhiro Hori, Ren Arita, Toshihiko Shimizu, Kohei Yamanoi, Kohei Sakai, Tomoharu Nakazato,

Nobuhiko Sarukura, Tsuguo Fukuda, Mitsuru Nagasono, Tadashi Togashi, Takahiro Sato and Tetsuya Ishikawa

Institute of Laser Engineering, Osaka University, Osaka, Japan

PS-15 Large Dependency of Oxide Band Edges on Surface Structures

Seungchul Kim, Chan-Woo Lee and Andrew M. Rappe

Center for Computational Science, Korea Institute of Science and Technology, Seoul, Korea

PS-16 First-Principles Molecular Dynamics Simulation Using Parallelized TOMBO: 2H + CO₂ Yielding HCOOH

M. Ikeoka and K. Ohno

Department of Physics, Yokohama National University, Kanagawa, Japan

PS-17 Computational Study on 0D, 1D and 2D Lattice Defects in Vanadium Hydrides

Hiroshi Ogawa

National Inst. of Advanced Industrial Science and Technol. (AIST), Ibaraki, Japan

PS-18 Light Elements Dissolved in α Iron: a First-Principles Study

Souissi Maaouia, Chen Ying and Numakura Hiroshi

Department of Materials Science, Graduate School of Engineering, Osaka Prefecture University, Osaka, Japan

PS-19 First-Principles Study of Phase Stability in Dilute Si-Doped α-Fe

Arkapol Saengdeejing, Ying Chen, Ken Suzuki, Hideo Miura, Tetsuo Mohri

Fracture and Reliability Research Institute, Graduate School of Engineering, Tohoku University, Miyagi, Japan

PS-20 Electronic Properties of Single Tetrapod-Shaped CdTe and CdTe/CdSe Nanocrystal Measured in STM.

A.S. Trifonov, R.B. Vasiliev, I.S. Ezubchenko, M.S. Sokolikova, D.R. Britov, D.E. Presnov,
O.V. Snigirevd and R. Belosludov

Lomonosov Moscow State University, Skobeltsyn Institute of Nuclear Physics, Moscow, Russia

PS-21 On Smoothing of the Potential Landscape of the Ising Models with Random Coupling Constants

K. Shida and Y. Kawazoe
Institute for Materials Research, Tohoku University, Miyagi, Japan

PS-22 Magnetic Properties of Endohedral Metallofullerenes Based on Nitride

Mixed Metal Cluster within Fullerene Cage with Trifluoromethyl Groups

<u>Atsushi Suzuki</u> and Takeo Oku

Department of Materials Science, The University of Shiga Prefecture, Shiga, Japan

PS-23 Fabrication, Micro Structures and Photovoltaic Properties of Poly(Copper Phthalocyanine)-Based Solar Cells

Makoto Iwase, Atsushi Suzuki, Tsuyoshi Akiyama and Takeo Oku

Department of Materials Science, The University of Shiga Prefecture, Shiga, Japan

PS-24 Fabrication, Nanostructures and Photovoltaic Properties of Polysilane-Based Solar Cells

Takeo Oku, Junya Nakagawa, Makoto Iwase, Kazumi Yoshida, Atsushi Kawashima,

Atsushi Suzuki, Tsuyoshi Akiyama, Katsuhisa Tokumitsu, Masahiro Yamada and Mika Nakamura

Department of Materials Science, The University of Shiga Prefecture, Shiga, Japan

PS-25 Fabrication, Nanostructures and Photovoltaic Properties of Silicon Phthalocyanine Based Solar Cells

Satoru Hori, Takeo Oku, Atsushi Suzuki, Tsuyoshi Akiyama and Yasuhiro Yamasaki

Department of Materials Science, The University of Shiga Prefecture, Shiga, Japan

PS-26 Nanostructure Characterization and Properties of Spherical Silicon Solar Cells

Masato Kanayama, Takeo Oku, Tsuyoshi Akiyama, Youichi Kanamori,
Yoshimasa Ohnishi, Yoshikazu Ohtani and Mikio Murozono
Department of Materials Science, The University of Shiga Prefecture, Shiga, Japan

PS-27 Prediction and Analysis of the Cathode Catalyst Layer Performance of Proton

Exchange Membrane Fuel Cells using Artificial Neural Network and Statistical Methods

S. Ahadian, N. Khajeh-Hosseini-Dalasm, K. Fushinobu, K. Okazaki and Y. Kawazoe

Institute for Materials Research, Tohoku University, Miyagi, Japan

WPI-Advanced Institute for Materials Research, Tohoku University, Miyagi, Japan

PS-28 Mechano-Chemical Reactions on Copper Chemical Mechanical Polishing

Processes Studied by Quantum Chemical Molecular Dynamics Simulations

Kentaro Kawaguchi, Takeshi Ishikawa, Yuji Higuchi, Nobuki Ozawa and Momoji Kubo

Fracture and Reliability Research Institute, Graduate School of Engineering, Tohoku University, Miyagi, Japan

PS-29 Chemical Degradation Process of Nafion Main Chain Studied by

First-Principles Molecular Dynamics Simulations

Akira Kobayashi, Takeshi Ishikawa, Yuji Higuchi, Nobuki Ozawa and Momoji Kubo

Fracture and Reliability Research Institute, Graduate School of Engineering, Tohoku University, Miyagi, Japan

PS-30 Low Friction Mechanism of Carbon Nitride Coatings Based on First-Principles

Molecular Dynamics and Tight-Binding Quantum Chemical Molecular Dynamics Methods

Seiichiro Sato, Shandan Bai, Takeshi Ishikawa, Yuji Higuchi, Nobuki Ozawa,

Koshi Adachi, Jean-Michel Martin and Momoji Kubo

Fracture and Reliability Research Institute, Graduate School of Engineering, Tohoku University, Miyagi, Japan

PS-31 Plasma Etching Processes Simulation of Gallium Nitride by Quantum Chemical Molecular Dynamics Study

Kazuyuki Yanagiya, Hiroshi Ito, Takuya Kuwahara, Takeshi Ishikawa,

Yuji Higuchi, Nobuki Ozawa and Momoji Kubo

Fracture and Reliability Research Institute, Graduate School of Engineering, Tohoku University, Miyagi, Japan

PS-32 Computational Simulation on Chemical Mechanical Polishing of Glass Surface by CeO₂ Abrasive Grain

Nobuki Ozawa, Kentaro Kawaguchi, Miho Nakamura, Takeshi Ishikawa, Yuji Higuchi and Momoji Kubo

Fracture and Reliability Research Institute, Graduate School of Engineering, Tohoku University, Miyagi, Japan

PS-33 Silicon Single-Electron Transistor with Suspended Island.

V.A. Krupenin, D.E. Presnov, S.V. Amitonov, K.V. Rudenko, V.I. Rudakov and A.S. Trifonov

 $Laboratory\ of\ Cryoelectronics,\ Faculty\ of\ Physics,\ M.V. Lomonosov\ Moscow\ State\ University,\ Moscow,\ Russian Conference of Cryoelectronics and Cryoelectronics and Cryoelectronics and Conference of Cryoelectronics and Cryoelec$

PS-34 The study of Atomic Force Microscopy by computer simulation

Nobuyuki Imahashi, Yasuhiro Senda, Shuji Shimamura, Janne Blomqvist and Risto Nieminem

Yamaguchi University, Yamaguchi, Japan

PS-35 User Interface for Calculation of Actinide Compound Properties Interface of Computer Programs for ACTInide

Science (ICP-ACTI)

Kenji Konashi, Kazuo Minato, Tomohiro Kabashima and Satoshi Minamoto

Institute for Materials Research, Tohoku University, Miyagi, Japan

PS-36 Tersoff Potential Investigation on Grain Boundaries in Multicrystalline Silicon

Hiroshi Mizuseki, Ryoji Sahara and Yoshiyuki Kawazoe

Institute for Materials Research, Tohoku University, Miyagi, Japan

PS-37 Micromagnetic Simulations on Hard and Soft Magnetic Granular Materials

Hiroshi Mizuseki, Kazuhito Shida, Ryoji Sahara and Yoshiyuki Kawazoe

Institute for Materials Research, Tohoku University, Miyagi, Japan

PS-38 Atomistic Level Description of Ni Amorphous Solid
<u>R. V. Belosludov</u>, D. V. Louzguine-Luzgin, A. Inoue, H. Mizuseki and Y. Kawazoe
Institute for Materials Research, Tohoku University, Miyagi, Japan

PS-39 Study of Electronic Structure and Thermoelectric Properties on Ba-Ga-Sn Clathrates

K. Akai, Y. Kono, K. Kishimoto, S. Yamamoto and S. Shimamura

Yamaguchi University, Yamaguchi, Japan

PS-40 First principles calculation of the enhanced conductivity of MnO_2 by Au-doping <u>L.J. Kang</u>, J.L. Kang, M.W. Chen, H. Mizuseki and Y. Kawazoe WPI-Advanced Institute for Materials Research, Tohoku University, Miyagi, Japan

PS-41 Efficient Self-Consistent GW Program Based on the All-Electron Mixed Basis Approach

Riichi Kuwahara, Yoshifumi Noguchi and Kaoru Ohno
Department of Physics, Yokohama National University, Kanagawa, Japan
Accelrys K K Tokyo Janan

PS-42 Theoretical and Computational Studies on Bi₂Se₃ as a Topological Insulator

<u>Ahmad Ranjbar</u>, Hiroshi Mizuseki and Yoshiyuki Kawazoe

Institute for Materials Research, Tohoku University, Miyagi, Japan

PS-43 Statistical-Thermodynamics Modeling for Ozone hydrate Phase Equilibria

<u>Hironori Nagashima</u>, Sanehiro Muromachi and Ryo Ohmura

Department of Mechanical Engineering, Keio University, Kanagawa, Japan

PS-44 Vibrational Spectra of Amyl-Alcohol Molecules in Clathrate Hydrates from *Ab initio* Molecular Dynamics Simulation

Masaki Hiratsuka, Ryo Ohmura, Amadeu K. Sum and Kenji Yasuoka

Department of Mechanical Engineering, Keio University, Kanagawa, Japan

PS-45 Carrier Concentration-Dependent Thermoelectric Properties of Titanium Dioxide from Boltzmann Transport Calculations

Ming Zhang, Kaoru Ohno and Lei Miao

Department of Physics, Graduate School of Engineering, Yokohama National University, Kanagawa, Japan

PS-46 Band Gap Engineering of Buckled Zigzag Nanoribbons with Perpendicular Electric Fields: a Theoretical Study

<u>Y. Liang</u>, V. Wang, H. Mizuseki and Y. Kawazoe

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