

LIST OF POSTER PRESENTATIONS

February 10, 2012 Fri. 17:30-19:00

- PS-1 Empirical Potential Investigation on Grain Boundaries in Multicrystalline Silicon
Hiroshi Mizuseki, Ryoji Sahara and Yoshiyuki Kawazoe
Institute for Materials Research (IMR), Tohoku University, Sendai, Japan
- PS-2 Micromagnetic Modelling of Granular Materials
Hiroshi Mizuseki, Kazuhito Shida, Ryoji Sahara and Yoshiyuki Kawazoe
Institute for Materials Research (IMR), Tohoku University, Sendai, Japan
- PS-3 Complexation Ability of Macrocyclic Cucurbituril Host with Pt - Anticancer Guests
N. S. Venkataramanan, H. Nejo, H. Mizuseki and Y. Kawazoe
Institute for Materials Research (IMR), Tohoku University, Sendai, Japan
- PS-4 Novel electric field effects on magnetic oscillations in graphene nanoribbons
Ning Ma
Department of Applied Physics, Xi'an Jiaotong University, Xi'an, China
- PS-5 Anomalous Valley Magnetic Moment of Graphene
Daqing Liu
Department of Applied Physics, Xi'an Jiaotong University, Xi'an, China
- PS-6 Study on the relationship between Curie temperature and effective exchange parameter in iron and its alloys
Takashi Shigematsu, Jian-Tao Wang, Alberto Martinez-Limia, Lothar Kunz, Thomas Eckl, Ryoji Sahara, Hiroshi Mizuseki and Yoshiyuki Kawazoe
Research and Technology Center Asia Pacific, District Japan, Bosch Corporation
- PS-7 First-principles study of intrinsic defect properties in hexagonal BN layer
W. Wang, N. Ma, H. Mizuseki and Y. Kawazoe
Institute for Materials Research (IMR), Tohoku University, Sendai, Japan
- PS-8 Electroluminescence of single CdSe nanocrystals induced by scanning tunneling microscope
Trifonov A.S., Osad'ko I.S., Ezubchenko I.S., Prokhorova I.G., Snigirev O.V., Nejo H.
National Institute for Materials Science (NIMS), Tsukuba, Japan
- PS-9 Suspended Silicon Nanowire Transistor High Sensitive Charge Sensor
V. A. Krupenin, D. E. Presnov, S. V. Amitonov, H. Nejo
National Institute for Materials Science (NIMS), Tsukuba, Japan

- PS-10 *Ab initio* Study of Na-doped $\text{CuIn}_{0.5}\text{Ga}_{0.5}\text{Se}_2$ Under High Pressure
P. Pluengphon, T. Bovornratanaraks, S. Vannarat and U. Pinsook
Large-Scale Simulation Research Laboratory, National Electronics and Computer Technology Center,
Pathumthani, Thailand
- PS-11 Formation mechanism of one-dimensional uneven peanut-shaped C_{60} polymer
A. Takashima, T. Nishii and J. Onoe
Tokyo Institute of Technology
- PS-12 One-dimensional ferromagnetism in graphene nanoribbon with grain boundaries
Jian Zhou, Ting Hu, and Jinming Dong
National Laboratory of Solid State Microstructures and Department of Material Science and Engineering,
Nanjing University, Nanjing, P. R. China
- PS-13 The transport properties of Silicene on ZnS film
Y. Y. Liang, H. Mizuseki and Y. Kawazoe
Institute for Materials Research (IMR), Tohoku University, Sendai, Japan
- PS-14 ZnO scintillator as High Spatial In situ imaging for Soft X-ray Laser
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-15 Heating-up and cooling-down molecular-dynamics simulations of 90-degree domain structures in PbTiO_3
Takeshi Nishimatsu, Kenta Aoyagi, Takanori Kiguchi, Toyohiko J. Konno, Yoshiyuki Kawazoe, Anil Kumar,
and Umesh V. Waghmare
Institute for Materials Research (IMR), Tohoku University, Sendai, Japan
- PS-16 Argon + Hydrogen mixed clathrate hydrate: molecular modeling
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Yoshiyuki Kawazoe
Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia
- PS-17 Dynamical properties of amorphous ices within lattice dynamics approach
Kirill V. Gets, Oleg S. Subbotin, Vladimir R. Belosludov
Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia
- PS-18 Thermodynamic stability of mixed ozone-containing hydrates
O. S. Subbotin, V. R. Belosludov, R. V. Belosludov, H. Mizuseki, Y. Kawazoe
Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia

- PS-19 First principles calculations on intrinsic point defects and related properties of langatate piezoelectric crystal
Chan-Yeup Chung, Ritsuko Yaokawa, Hiroshi Mizuseki and Yoshiyuki Kawazoe
Institute for Materials Research (IMR), Tohoku University, Sendai, Japan
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T. Suyama, T. Yanagida, Y. Yokota, A. Yoshikawa, M. Nagasono, Tetsuya Ishikawa
Institute of Laser Engineering, Osaka Univ., Osaka, Japan
- PS-21 First-principles study of frequency-dependent polarizabilities and Van der Waals dispersion coefficients for
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V. R. Belosludov, O. S. Subbotin, R. V. Belosludov, Y. Kawazoe
Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia
- PS-22 Study on the Luminescence and Energy Level of Rare Earth Ion Doped in APLF Glass Host
M. Tsuboi, M. Kouno, T. Nakazato, T. Shimizu, M. Cadatal-Raduban, K. Yamanoi, K. Sakai, R. Nishi,
Y. Minami, K. Takeda, Y. Arikawa, N. Sarukura, T. Norimatsu, M. Nakai, H. Azechi, T. Murata, S. Fujino,
H. Yoshida, T. Suyama, K. Fukuda, A. Yoshikawa, N. Sato, H. Kan, K. Kamada and Y. Usuki
Institute of Laser Engineering, Osaka Univ., Osaka, Japan
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Y. Senda, T. Tsukinari, S. Shimamura, J. Blomqvist and R. M. Nieminen
Department of Applied Science, Yamaguchi University, Yamaguchi-Ube, Japan
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Yoshifumi Noguchi, Osamu Sugino, Momoko Nagaoka, Soh Ishii, and Kaoru Ohno
Institute for Solid State Physics, The University of Tokyo, Chiba, Japan
- PS-25 Electron-transport properties of one-dimensional exotic- C_{60} polymer films
S. Ryuzaki, M. Nishiyama, A. Takashima, and J. Onoe
Tokyo Institute of Technology, O-okayama, Meguro, Tokyo
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Kohei Yamanoi, Yasunobu Arikawa, Tomoharu Nakazato, Marilou Cadatal-Raduban, Toshihiko Shimizu,
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Takahiro Murata, Kentaro Fukuda, Toshihisa Suyama, Akira Yoshikawa, Nakahiro Sato, Hirofumi Kan
Institute of Laser Engineering, Osaka University, Osaka, Japan
- PS-27 Development of all-electron mixed-basis *ab initio* program TOMBO and application for hydrogen storage
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Ryoji Sahara, Hiroshi Mizuseki, Marcel Sluiter, Kaoru Ohno, and Yoshiyuki Kawazoe
Institute for Materials Research (IMR), Tohoku University, Sendai, Japan

- PS-28 Modern molecular dynamic computing on GPU with NVidia CUDA and ATI OpenCL technologies in Atomic Simulation Environment (ASE)
Sergey V. Seriy
Education Ministry of Russian Federation ,Komsomolsk-on-Amur State Technical University, Russia
- PS-29 First principle investigation of the core/shell nano-precipitate in FeCuMnNiAl alloy
L. J. Kang, Y. R. Wen, M. W. Chen, H. Mizuseki, Y. Kawazoe
WPI-AIMR, Tohoku University, Sendai, Japan
- PS-30 High-pressure phase transitions of hydrogen cyanide and cyanogen molecules
Mohammad Khazaei and Yoshiyuki Kawazoe
Institute for Materials Research (IMR), Tohoku University, Sendai, Japan
- PS-31 Many-electron states of nitrogen-vacancy centers in diamond and spin density calculations
Ahmad Ranjbar, Mohsen Babamoradi, Mehdi Heidari Saani, Mohammad Ali Vesaghi, Keivan Esfarjani, and Yoshiyuki Kawazoe
Institute for Materials Research (IMR), Tohoku University, Sendai, Japan
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Takeshi Fujita and Hannes Raebiger
Department of Physics, Yokohama National University, Yokohama Japan
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S. Ahadian, N. Khajeh-Hosseini-Dalasm, K. Fushinobu, K. Okazaki, Y. Kawazoe
Institute for Materials Research (IMR), Tohoku University, Sendai, Japan
- PS-34 First-principles calculations and thermodynamic modeling of the Mg-B-C system
Arkapol Saengdeejing, James E. Saal and Zi-Kui Liu
Fracture and Reliability Research Institute, Tohoku University, Sendai, Japan
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Naoya Kiyokane and Tesuo Mohri
Division of Materials Science and Engineering, Graduate School of Engineering, Hokkaido University
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Yusuke Noda and Kaoru Ohno
Department of Physics, Yokohama National University, Yokohama, Japan
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R. V. Belosludov, A. A. Farajian, H. Mizuseki, K. Miki and Y. Kawazoe
Institute for Materials Research (IMR), Tohoku University, Sendai, Japan

- PS-38 Controlling Percolation by Modulating the Granular Size of Insulating Materials
K. Shida, R. Sahara, M.N. Tripathi, H. Mizuseki, and Y. Kawazoe
Institute for Materials Research (IMR), Tohoku University, Sendai, Japan
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Souissi Maaouia, Chen Ying, Numakura Hiroshi
Department of Materials Science, Graduate School of Engineering, Osaka Prefecture University,
Osaka, Japan
- PS-40 Quantum Monte Carlo study of molecular crystals
Kenta Hongo
Research and Development Center for Data Assimilation, The Institute of Statistical Mathematics,
Tokyo, Japan
- PS-41 LDA+U study of PuO₂ on ground state with spin-orbital coupling
Hao Wang and Kenji Konashi
International Research Center for Nuclear Materials Science, Institute for Materials Research,
Tohoku University, Ibaraki, Japan
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Masahiro Yamada, Mika Nakamura
Department of Materials Science, The University of Shiga Prefecture, Shiga, Japan
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Tomohiro Mori
Department of Materials Science, The University of Shiga Prefecture, Shiga, Japan
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A. Suzuki, T. Oku
Department of Materials Science, The University of Shiga Prefecture, Shiga, Japan
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Takeo Oku, Kazumi Yoshida, Takuma Yoshikawa, Atsushi Kawashima, Atsushi Suzuki, Tsuyoshi Akiyama,
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Department of Materials Science, The University of Shiga Prefecture, Shiga, Japan
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Fracture and Reliability Research Institute (FRRI), Graduate School of Engineering, Tohoku
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- PS-47 Nickel Nanoparticles Sintering Processes on YSZ and ScSZ Surface via Molecular Dynamics Simulation
Jingxiang Xu, Ryota Sakanoi, Yuji Higuchi, Nobuki Ozawa, Tomomi Shimazaki, Momoji Kubo
Fracture and Reliability Research Institute (FRRI), Graduate School of Engineering, Tohoku University,
Sendai, Japan
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Fracture and Reliability Research Institute (FRRI), Graduate School of Engineering, Tohoku University,
Sendai, Japan
- PS-49 The Chemical Aging Process of Polyethylene Studied by First-Principles and Coarse-Grained Molecular
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Fracture and Reliability Research Institute (FRRI), Graduate School of Engineering, Tohoku University,
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Leslie V. Woodcock
Manchester Interdisciplinary Biocentre, University of Manchester, UK and Department of Physics,
Kyonggi University, Suwon, S. Korea
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Fracture and Reliability Research Institute (FRRI), Graduate School of Engineering, Tohoku University,
Sendai, Japan
- PS-52 A fundamental study of hydrogen effect on alloy and oxide film surfaces
Nishith Kumar Das and Tetsuo Shoji
Fracture and Reliability Research Institute & New Industry Creation Hatchery Center, Tohoku
University, Sendai, Japan
- PS-53 Adsorption behavior of CO₂ on Li₂ZrO₃ surface from first-principles calculations
N.Tokuda, S. Ueda, R. Belosludov, Y. Kawazoe and T. Ariyama
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