# Poster Session 1 (Day 1)

**P-01 A molecular dynamics study on the molecular recognition and a challenge to drug design**

Takefumi Yamashita
The University of Tokyo

**P-02 Calculation of temperature dependent diffusion of H across Ni(111) using a novel ensemble potential energy surface approach**

A. R. Hopkinson and M. I. J. Probert
University of York

**P-03 Sacrificial Anion Reduction Mechanism for Electrochemical Stability Improvement in Highly Concentrated Li-salt Electrolyte**

Keitaro Sodeyama [A,B], Yuki Yamada [A,C], Atsuo Yamada [A,C], and Yoshitaka Tateyama [A,B,D]
Kyoto University [A)], NIMS [B)], The University of Tokyo [C)], JST-PRESTO and CREST [D)]

**P-04 Symplectic Time Integrator with Transformed Canonical Variables**

Atsushi M. Ito
National Institute for Fusion Science

**P-05 Double-QM/MM Method for Investigating Donor-Acceptor Electron Transfer in Solution**

Zdenek Futera [A,B,C], Keitaro Sodeyama [B,D], and Yoshitaka Tateyama [B,C,D,E]
Keio University [A)], NIMS [B)], CREST [C)], Kyoto University [D)], PRESTO, JST [E)]

**P-06 DFT-MD blue-moon ensemble study on reductive decomposition of carbonated-based solvent in lithium ion battery**

Yoshitaka Tateyama[A,B,C], Keisuke Ushirogata[D], Keitaro Sodeyama[A,B], & Yukihiro Okuno[D]
NIMS[A)], Kyoto University[B)], PRESTO, JST[C)], FUJIFILM Corporation[D)]

**P-07 Reaction between $CO_2$ and 2-Aminoethanol in Aqueous Solution**

Yoshiyuki Kubota[A], Toshiharu Ohnuma[B], and Tomáš Bučko[C]
The Kansai Electric Power Company., Inc. [A)], Central Research Institute of Electric Power Industry [B)], Comenius University [C)]

**P-08 Molecular Dynamics Simulation of Sum Frequency Generation Spectra at Water and Aqueous Surfaces**

Tatsuya Ishiyama [A] and Akihiro Morita [B]
University of Toyama [A)], Tohoku University[B)]

**P-09 Boundary based on exchange symmetry theory: A QM/MM method for open systems**

Motoyuki Shiga [A] and Marco Masia [B]
Japan Atomic Energy Agency [A)], University of Sassari [B)]

**P-10 Theoretical study of the molecular interactions in secondary structures of proteins**

Yu Takano[A,B], Ayumi Kusaka[A], and Haruki Nakamura[A]
Osaka University[A)], JST-CREST [B)]

**P-11 Universal Medium-Range Order of Amorphous Metal Oxides**

Kengo Nishio, Takehide Miyazaki and Hisao Nakamura
National Institute of Advanced Industrial Science and Technology (AIST)

**P-12 A characterization of the amorphous silica structure by persistent homology**

Takenobu Nakamura [A], Yasuaki Hiraoka [B], Akihiko Hirata [A], Emerson Escolor [B],
Kaname Matsue [C] and Yasumasa Nishiura [A]
Tohoku University [A)], Kyushu University [B)], The Institute of Statistical Mathematics [C)]

**P-13 Molecular Dynamics Study of Aggregation Mechanism of SDS Micelle**

Noriyuki Yoshii, Shinji Kawada, Kazushi Fujimoto, and Susumu Okazaki
Nagoya University

**P-14 Analysis for the structural stability of chignolin**

Yutaka Maruyama, and Ayori Mitsutake
Keio University

**P-15 Phase Diagram for a Lennard-Jones System Obtained through Constant-Pressure Molecular Dynamics Simulations**

Yosuke KATAOKA[A] and Yuri YAMADA[B]
Hosei University [A)], Tokyo Denki University[B)]

**P-16 Monte Carlo simulation of chiral liquid crystals with large pitch distances**

Paul Brumby and Kenji Yasuoka
Keio University

**P-17 Melting phenomena of the modified Lennard-Jones system**

Yuta Asano [A], Kazuhiro Fuchizaki [B], and Nobuyasu Ito [A, C]
RIKEN AICS [A)], Ehime University [B)], The University of Tokyo [C)]

**P-18 Potential Development of Borate Crystals, Glasses and Melts Based on First-Principles Calculation**

Yoshiki Ishii [A], Kohei Kasahara [A], Norikazu Ohtori [A], Koichi Shiraki [B],Mathieu Salanne [C], and Paul A. Madden[D]
Niigata University [A)], Nippon Sheet Glass Co. Ltd. [B)], UPMC Univ Paris 06 and CNRS [C)], University of Oxford [D)]

**P-19 Concentration Dependency Research of Amyloid-Forming Peptides by Using Molecular Dynamics Simulations**

Naohiro NISHIKAWA [A,B], Yoshitake SAKAE [A], and Yuko OKAMOTO [A,]
Nagoya Univ. [A)], Institute for Molecular Science [B)]

**P-20 Photophysics of fulvene under the non-resonant Stark effect. Shaping the conical intersection seam**

Sergi Ruiz-Barragan and Lluis Blancafort
Universitat de Girona

**P-21 Random Matrix Theory and Higher Order Principal Component Analysis of Protein-Ligand Interaction by Molecular Dynamics Simulation**

Masanori Yamanaka
Nihon University

**P-22 Two-Temperature Langevin Dynamics in Laser-Ablated Metals**

Yasushi Takéuchi [A], Atsushi Sunahara [A], and Katsunobu Nishihara [B]
Institute for Laser Technology [A)], Osaka University [B)]

**P-23 Mass scaling in replica-exchange method with the Nosé-Hoover thermostat**

Tetsuro Nagai and Takuya Takahashi
Ritsumeikan University

**P-24 Multiscale model for AFM using MD/continuum coupling method**

Yasuhiro Senda [A], Shuji Shimamura [A], Janne Blomqvist [B] and Risto Nieminen [B]
Yamaguchi Univ. [A)], Aalto Univ. [B)]

**P-25 $\mu^2$lib: a library for developing multicopy and multiscale molecular dynamics simulation programs**

Tohru Terada [A], Kei Moritsugu [B], Yasuhiro Matsunaga [C], and Akinori Kidera [B]
The University of Tokyo [A)], Yokohama City University [B)], RIKEN [C)]

**P-26 Dimerization of A $\beta$ fragments by the Hamiltonian replica-permutation method**

Satoru G. Itoh [A,B] and Hisashi Okumura [A,B]
Institute for Molecular Science [A)], The Graduate University of Advanced Studies [B)]

**P-27 Molecular Dynamics Simulation of Shiga Toxin**

Kazumi Omata [A], Yoshiharu Mori [B], Hisashi Okumura [B,C], and Kiyotaka Nishikawa [D]
National Center for Global Health and Medicine [A)], Institute for Molecular Science [B)],
The Graduate University for Advanced Studies [C)], Doshisha University [D)]

**P-28 Metadynamics Study on Z/E-Thermal Isomerization of Azobenzenes under high pressure**

Y. Shigemitsu[1,2] and Y. Ohga[3]
[1]Industrial Technology Center of Nagasaki, [2]Nagasaki University, [3]Oita University

**P-29 Huge-Scale Molecular Dynamics Simulation of Multi-bubble Nuclei**

Hiroshi Watanabe
The University of Tokyo

**P-30 Theoretical design of novel copper doped gold cluster by Car-Parrinello molecular dynamics**

Kenichi Koizumi [A,B], Mauro Boero [C], and Katsuyuki Nobusada [C]
IMS [A)], ESICB [B)], IPCMS [C)]

**P-31 Free energy surface of Water Confined in Slit Pores**

Toshihiro Kaneko[1], Jaeil Bai[2], Kenji Yasuoka[3], Ayori Mitsutake[3] and Xiao Cheng Zeng[2]
[1]Tokyo University of Science, [2] University of Nebraska-Lincoln, [3]Keio University

**P-32 Thermal Stability of Gramicidin A in Lipid Bilayer: A Free Energy Analysis**

Hiroaki Saito
Kanazawa University

**P-33 Energy Landscape of All-atom Protein-protein Interactions Revealed by Multiscale Enhanced Sampling**

Kei Moritsugu[A*], Tohru Terada[B], and Akinori Kidera[A]
Yokohama City University [A)], The University of Tokyo [B)]

**P-34 Molecular Dynamics Simulation of Pool Boiling of a Lennard-Jones Liquid**

Hajime Inaoka [A] and Nobuyasu Ito [B,A]
RIKEN [A)], The University of Tokyo [B)]

**P-35 Preference of Water and Methanol Molecules Flowing into Carbon Nanotubes under Influence of Electric Field**

Winarto, Daisuke Takaiwa, Eiji Yamamoto, and Kenji Yasuoka
Keio University

# Poster Session 2 (Day 2)

**P-36 Alchemical free energy calculation for theophylline-RNA aptamer complex**
Yoshiaki Tanida and Azuma Matsuura
Fujitsu Laboratories Ltd.

**P-37 Dissociation Free-Energy Profiles of Specific and Nonspecific DNA−Protein Complexes**
Yoshiteru Yonetani
Japan Atomic Energy Agency

**P-38 Comparison of conserved water molecules in rhodopsin and opsin: Molecular dynamics study**
Katsufumi Tomobe[A], Eiji Yamamoto[A], Kholmirzo Kholmurodov[B] and Kenji Yasuoka[A]
Keio University[A)], Joint Institute for Nuclear Research[B)]

**P-39 Nonequilibrium molecular dynamics simulations of amyloid fibril disruption by ultrasonic cavitation**
Hisashi Okumura [A,B] and Satoru G. Itoh [A,B]
Institute for Molecular Science[A)], The Graduate University for Advanced Studies[B)]

**P-40 Molecular dynamics study of glycolipids/lipids membrane with Coarse-Grained Model**
Kento Inoue, Daisuke Takaiwa , Kenji Yasuoka, and Masuhiro Mikami
Keio University

**P-41 Numerical assessments of the replica-permutation molecular dynamics with and without detailed balance condition**
Hiroaki Nishizawa [A] and Hisashi Okumura [A,B]
Institute for Molecular Science[A)], The Graduate University for Advanced Studies[B)]

**P-42 Sparse representation for a potential energy surface**
Atsuto Seko, Akira Takahashi and Isao Tanaka
Kyoto University

**P-43 Effect of electrodes as a device of extended environment on electrostatics**
Nobuyuki Takahashi
Hokkaido University of Education

**P-44 The water model dependency of the melting point of hexagonal ice**
Daisuke Takaiwa [A], Ryuji Sakamaki [A], Amadeu K. Sum [B], Tetsu Narumi [C], and Kenji Yasuoka[A]
Keio University[A)], Colorado School of Mines[B)], University of Electro-Communications[C)]

**P-45 Membrane Fusion: Free Energy Analysis**
Wataru Shinoda [A], Shuhei Kawamoto [A, B], and Michael L. Klein [B]
Nagoya University[A)], Temple University[B)]

**P-46 New code for phonon anharmonic effects analysis of MD trajectories**
Abel Carreras, Atsushi Togo, and Isao Tanaka
Kyoto University

**P-47 Systematic first-principles lattice thermal conductivity calculations**
Atsushi Togo and Isao Tanaka
Kyoto University

**P-48 Searching of the dense packing state of hard-sphere systems by using the Wang-Landau sampling**

Tomoaki Nogawa
Toho University

**P-49 Molecular dynamics simulation study of helium diffusion behavior in defective tungsten material**

A. Takayama [A], A. M. Ito [A], Y. Oda [A], and H. Nakamura [A,B]
National Institute for Fusion Science [A)], Nagoya University [B)]

**P-50 Evaluation of the thermal motion of the hydrogen bonds in cellulose crystals using Car-Parrinello molecular dynamics simulation**

Daichi HAYAKAWA [A], Kazuyoshi UEDA [A], Karim MAZEAU [B]and Yoshiharu NISHIYAMA[B]
Yokohama National University [A)], CERMAV, CNRS [B)]

**P-51 Connectivity Altering Monte Carlo - An Accurate and Effective Sampling Method for Polymer Melts**

Krzysztof Moorthi[A], Kazunori Kamio[B], Javier Ramos[C] and Doros N. Theodorou[D]
[A)] Mitsui Chemicals, Inc., [B)]MC Analysis and Consulting Service, [C)] IEM CSIC, [D)] National Technical University of Athens

**P-52 Structural analysis of telechelic polymer solution using dissipative particle dynamics simulations**

Noriyoshi Arai
Kinki University

**P-53 Stable and Efficient Linear Scaling First-Principles Molecular Dynamics for 10,000+ atoms**

M. Arita [A,B], D. R. Bowler [C,D, E], and T. Miyazaki [A,B]
Tokyo University of Science [A)], National Institute for Materials Science (NIMS) [B)], University College London (UCL) [C)], London Centre for Nanotechnology, UCL [D)], International Center for Materials Nanoarchitectonics (MANA), NIMS [E)]

**P-54 Development of variational path integral molecular dynamics method with applications to molecular systems**

Shinichi Miura
Kanazawa University

**P-55 Replica deterministic exchange molecular dynamics and its application to biomolecular simulations**

Ryo URANO and Yuko OKAMOTO
Nagoya University

**P-56 Extended Study on Molecular Dynamics of Methane Hydrate Nucleation**

D. Yuhara [A], D. Suh [A], B.C. Barnes [B], D.T. Wu [B], A.K. Sum [B], and K. Yasuoka [A]
Keio University [A)], Colorado School of Mines [B)]

**P-57 DFT study of $Ti^{3+}$ states near oxygen vacancy on $TiO_2$ (110): a new interpretation of STM**

Taizo Shibuya [A], Kenji Yasuoka [A], Susanne Mirbt [B] and Biplab Sanyal [B]
Keio University [A)], Uppsala University [B)]

**P-58 Simulated Tempering Molecular Dynamics Simulations using the Metropolis, Heat bath, or Suwa-Todo Algorithm**

Yoshiharu Mori [A] and Hisashi Okumura [A,B]
Institute for Molecular Science [A)], The Graduate University for Advanced Studies [B)]

**P-59 On the comparison of different barostat implementations for the prediction of the breathing behavior in MIL-53 frameworks**

S. Rogge[A], L. Vanduyfhuys[A], T. Verstraelen[A], G. Maurin[B], and V. Van Speybroeck[A]
Ghent University [A)], Institut Charles Gerhardt Montpellier [B)]

**P-60 Coarse-grained model of membrane protein**

Shuhei Kawamoto [A,B], Giacomo Fiorin [A], Chris MacDeraid [A], Russell Devane [C], Wataru Shinoda [B], and Michael L. Klein [A]
Temple University [A)], Nagoya University [B)], P&G [C)]

**P-61 Properties and perspectives of first-principles logarithmic mean force dynamics**

Tatsuki Oda [A], Makoto Nakamura [A], Masao Obata [A], and Tetsuya Morishita [B]
Kanazawa University [A)], AIST [(B)]

**P-62 Pressure and temperature controlling in generalized isobaric-isothermal ensembles**

Hideo Doi and Kenji Yasuoka
Keio University

**P-63 The effects of handling coulomb interaction on transport characteristic of liquid crystal system**

Takuma Nozawa [A], Kazuaki Takahashi [A], Tetsu Narumi [B] and Kenji Yasuoka [A]
Keio University [A)], University of Electro-Communications [B)]

**P-64 Vibrational spectra of alcohol molecules in clathrate hydrates**

Masaki Hiratsuka [A], Ryo Ohmura [A], Amadeu K. Sum [B], Saman Alavi [C], and Kenji Yasuoka [A]
Keio University [A)], Colorado School of Mines [B)], National Research Council of Canada [C)]

**P-65 Development of Machine-Learning-Based Interatomic Potential**

Ryo KOBAYASHI, Tomoyuki TAMURA, and Shuji OGATA
Nagoya Institute of Technology

**P-66 Synchronized molecular dynamics simulation via macroscopic heat and momentum transfer for polymer lubrications**

Shugo YASUDA [A] and Ryoichi YAMAMOTO [B]
University of Hyogo [A)], Kyoto University [B)]

**P-67 Density of States for 2D Ising Model**

Hisashi Shimizu and Gaku Fukunaga
Shinshu University

**P-68 Origin of *1/f* fluctuations of number of water molecules on lipid membrane surfaces**

Eiji Yamamoto, Takuma Akimoto, Masato Yasui, and Kenji Yasuoka
Keio University

**P-69 Finite-Precision Periodic Orbits, Thermodynamics, Boltzmann's Constant, and Nonequilibrium Entropy**

Carol Griswold Hoover and William Graham Hoover
Ruby Valley Research Institute

**P-70 Applicability of Kelvin Equation to Vapor-Liquid Coexistence of Water in Nanocylinder**

Toshiki Mima[A], Ikuya Kinefuchi[A], Yuta Yoshimoto[A], Akinori Fukushima[B], Takashi Tokumasu[C], Shu Takagi[A], and Yoichiro Matsumoto[A]
The University of Tokyo[A)], Tokyo University of Agriculture and Technology[B)], Tohoku University[C)]