3rd International Conference on Molecular Simulation (ICMS2013)

The date of presentation is given at the first number.
Underlined is the presenter among more than one authors.
Candidates for student award is marked with ☆ in front of the poster title.

Day 1 Nov. 18

9:00−9:10

Opening Address by Conference Chair
Shiaki Hyodo

President of the Molecular Simulation Society of Japan
Susumu Okazaki

chair: Susumu Okazaki

9:10 **PL1** **Structure, Dynamics, and Thermodynamic Stability of High Pressure Ices and Clathrate Hydrates**
Hideki Tanaka

9 : 55 break

10:10−11:40 **Oral**

chair: Pavel Jungwirth

10:10 **1O01** **Low-density liquid water is the mother of ice: on the relation between liquid structure, thermodynamics and ice crystallization**
Valeria Molinero

10:40 **1O02** **Molecular Simulation of Confined Water and Aqueous Solution**
Kenji Yasuoka

11:10 **1O03** **Structure and Dynamics of Nanoconfined Liquids**
Ward H. Thompson

11 : 40 break

11:55−12:55 **Oral**

chair: Kenji Yasuoka

11:55 **1O04** **Molecular Simulation for Liquid Interfaces**
Akihiro Morita

12:25 **1O05** **Motion of H^+ in H-bond Network: From Quantum Confinement to Fermi Resonance**
Jake Tan, Chen-Wei Tsai, Jer-Lai Kuo

12 : 55 lunch

13:45−14:45 **Poster**

14:45−16:15 **Oral**

chair: Jeffery B. Klauda

14:45 **1O06** **Interactions Between Ions and Proteins in Water: The Hofmeister Series**
Pavel Jungwirth

15:15 **1O07** **Urea-induced denaturation of $PreQ_1$-riboswitch**
Changbong Hyeon

15:45 **1O08** **Biomolecular Simulations under Cellular Crowding Environment**
Yuji Sugita, Ryuhei Harada, Isseki Yu, Takahru Mori, Jaewoon Jung, Michael Feig

16 : 15 break

16:30−18:00 **Oral**

chair: Wataru Shinoda

16:30 **1O09** **Free-Energy Analysis of Water Affinity in Polymer Studied by Atomistic MD and the Energy-Representation Method**
Tomonori Kawakami, Masahiro Kitabata, Isamu Shigemoto

17:00 **1O10** **Force Fields and Simulation Protocols in Predictions of Adsorption**
Huai Sun

17:30 **1O11** **Free-Energy Analysis of Solvation and Membrane Effects on Protein Configurations**
Nobuyuki Matubayasi

Day 2 Nov. 19

chair: Yuko Okamoto

9:00 **PL2** **Capturing pH mediated physics and chemistry in biological systems**
Charles L. Brooks III

9 : 45 break

10:00−11:30 **Oral**

chair: Mitsunori Ikeguchi

10:00 **2O01** **Large-Scale and All-Atom Molecular Dynamics Simulation of Viruses Using the K Computer**
Susumu Okazaki

10:30 **2O02** **Simulations of Biomembranes: Importance of Lipid Diversity and Structural Changes of Membrane Transport Proteins**
Jeffery B. Klauda

11:00 **2O03** **Structure and function of the transmembrane domain of Amyloid Precursor Protein and its role in the amyloid β protein aggregation pathway**
Laura Dominguez, Leigh Foster, D. Thirumalai, John E. Straub

11 : 30 break

11:45–12:45 **Oral**

chair: Changbong Hyeon

11:45 **2O04** **Molecular recognition by intrinsically disordered proteins – insights from molecular simulation**
David de Sancho, Michael Knott, Christopher M. Baker, Robert B. Best

12:15 **2O05** **Dynamics of Neuraminidase: from Hamiltonian REMD to novel inhibitor design**
Nanyu Han, Yuguang Mu

12 : 45 lunch

13:45–14:45 **Poster**

14:45–16:15 **Oral**

chair: Yuji Sugita

14:45 **2O06** **Combination of MD and SAXS to Explore Protein Dynamics**
Mitsunori Ikeguchi

15:15 **2O07** **Molecular simulation of protein folding, conformational change and self-assembly**
Peter G. Bolhuis

15:45 **2O08** **Generalized-ensemble algorithms for molecular simulations**
Yuko Okamoto

16:30 **Excursion Visit to K Computer**

18:45 **Banquet with Bay Cruise (Transportation bus departs at 18:00)**

Day 3 Nov. 20

chair: Shiaki Hyodo

9:00 **PL3** **Chemical Reaction Rates from Ring Polymer Molecular Dynamics**
David E. Manolopoulos

9 : 45 break

10:00–11:30 **Oral**

chair: Akihiro Morita

10:00 **3O01** **Variational path integral molecular dynamics with applications to molecular systems**
Shinichi Miura

10:30 **3O02** **Learning chemistry from multiple first-principles simulations**
Giovanni La Penna

11:00 **3O03** **Molecular Statistical Mechanics of Chemical Reactions in Solution Phase**
Hirofumi Sato

11：30 break

11:45−12:45 Oral

chair: Ward H. Thompson

11:45 **3O04** **Crucial Role of Protein Flexibility in Enzymatic Catalysis**
Shigehiko Hayashi

12:15 **3O05** **Massively Parallel Implementation of the QM/MM Approach Combined with a Theory of Solutions**
Hideaki Takahashi, Yuji Miki, Akihiro Morita

12：45 lunch

13:45−14:45 Poster

14:45−16:45 Oral

chair: Mitsuhiro Matsumoto

14:45 **3O06** **Smoothed Profile Method for DNS of Particle Dispersions**
Ryoichi Yamamoto, John J. Molina

15:15 **3O07** **Balance of Enthalpy and Entropy in Depletion Forces**
Liel Sapir, Shahar Sukenik, Daniel Harries

15:45 **3O08** **Mechanical stability of proteins: from coarse-grained to all-atom simulations**
Mai Suan Li, Maksim Kouza

16:15 **3O09** **Free Energy Analysis of Topological and Morphological Changes in Lipid Membranes: Molecular Dynamics Study**
Wataru Shinoda, Shuhei Kawamoto

16：45 break

chair: Nobuyuki Matubayasi

16:55 **MSSJ Award Lecture: Effective sampling algorithms and analysis methods for protein simulations**
Ayori Mitsutake

17:30 **Closing Remarks**
Shiaki Hyodo

17:35 **Business Meeting of the Molecular Simulation Society of Japan (in Japanese)**

Poster day 1

1P01 **Coupled-Cluster Calculations on Electronic Circular Dichroism of Single and Double Helicenes**
Ikenosako Mina, Takeharu Kusuki, Yoshito Nakai, Yoshihisa Inoue, Tadashi Mori

1P02 **Fluctuation Flooding Method (FFM) for enhancing conformational sampling of proteins**
Ryuhei Harada, Yu Takano, Yasuteru Shigeta

1P03 **Multiscale enhanced sampling and its applications to large solvated proteins**
Kei Moritsugu, Tohru Terada, Akinori Kidera

1P04 **Drug export process of MATE multidrug efflux transporter by Molecular dynamics simulations**
Wataru Nishima, Yoshiki Tanaka, Ryuichiro Ishitani, Osamu Nureki, Yuji Sugita

1P05 **Effects of Initial Settings on Computational Protein-Ligand Docking Accuracies for several Docking Programs**
Akifumi Oda, Noriyuki Yamaotsu, Shuichi Hirono, Yurie Watanabe, Shuichi Fukuyoshi, Ryoichi Nakagaki, Ohgi Takahashi

1P06 **Logarithmic Mean-Force Dynamics (LogMFD): Application to a Model System of Protein-G**
Tetsuya Morishita

1P07 **Molecular Dynamics Simulation Underlying the Early Stage of the Channelrhodopsin**
Mizuki Takemoto, Hideaki E. Kato, Michio Koyama, Jumpei Ito, Motoshi Kamiya, Shigehiko Hayashi, Andrés D. Maturana, Karl Deisseroth, Ryuichiro Ishitani, Osamu Nureki

1P08 **Study on the C-terminal domain of eukaryotic RNA polymerase II by using a molecular dynamics simulation**
Yasushige Yonezawa

1P09 **Prediction of Protein-ligand Binding Affinities Using Molecular Simulations**
Noriaki Okimoto, Atsushi Suenaga, Yoshinori Hirano, Makoto Taiji

1P10 ☆**Conversion of CO_2, CH_4 and C_2H_6 to Organic Compound on Ir-Graphene Oxide Surface - A First-Principle Investigation**
Chih-Chun Chen, Jia-Jen Ho

1P11 ☆**Molecular Dynamics Study on Simplified Model Membranes for Normal Murine Thymocytes and Leukemic GRSL Cell Plasma Membranes**
Soichiro Shibayama, Yoshimichi Andoh, Susumu Okazaki

1P12 **Conformational analysis of PA-glycans by replica-exchange molecular dynamics simulation.**
Shigehisa Watabe, Suyong Re, Wataru Nishima, Eiro Muneyuki, Yuji Sugita

1P13 **Molecular Dynamics Simulation of Enzyme-Substrate Analogue Complex of Heterotetrameric Sarcosine Oxidase**
Go Watanabe, Akinori Hiroshima, Haruo Suzuki, Shigetaka Yoneda

1P14 ☆**Electrostatic steering mechanism in selective binding of KIF1A on microtubule**
Yukinobu Mizuhara, Jun Ohnuki, Koji Umezawa, Takano Mitsunori

1P15 ☆**Piezoelectricity of protein and its implication for function**
Jun Ohnuki, Takato Sato, Koji Umezawa, Taro Q. P. Uyeda, Mitsunori Takano

1P16 **Nature of Proton Transport in Hydrocarbon Membranes for Fuel Cell Applications**
Yoong-Kee Choe, Eiji Tsuchida, Tamio Ikeshoji, Akihiro Ohira, Takahiro Ohkubo, Neil Henson, Yu Seung Kim

1P17 **Non-equilibrium Molecular Dynamics Simulations for Amyloid Disruption by Hypersonic Wave**
Hisashi Okumura, Satoru G. Itoh

1P18 **Large scale molecular dynamics simulations of vapour-to-liquid nucleation**
Jürg Diemand, Raymond Angelil, Kyoko K Tanaka, Hidekazu Tanaka

1P19 **Cation-π vs. Water-π : Theoretical analysis of structural stability of the active center of T1 lipase employing a novel accurate and efficient description of effective potential**
Atsushi Nakamura, Jiyoung kang, Masaru Tateno

1P20 **A reaction analysis for deprotonation of sulfonic group of perfluorosulfonic acid molecule in the low hydration level by density functional theory**
Hironori Sakai, Takashi Tokumasu

1P21 **Multiple length and time scales of dynamic heterogeneities in fragile and strong glass-forming liquids**
Kang Kim, Shinji Saito

1P22 **Molecular Dynamics Simulation for Phase Behavior of Bolaamphiphilic Solution**
Susumu Fujiwara, Takumi Miyata, Takashi Itoh, Masato Hashimoto

1P23 **Theoretical studies on the stability of clathrate hydrates**
Takato Nakayama, Masakazu Matsumoto, Hideki Tanaka

1P24 **Wetting Transition of Ethanol-Water Droplet on Smooth and Textured Surfaces**
Atanu K. Metya, Jayant K Singh

1P25 **Phase Transitions of Water Confined in Slit Pores**
Toshihiro Kaneko, Jaeil Bai, Kenji Yasuoka, Ayori Mitsutake, Xiao Cheng Zeng

1P26 **The channel size dependence of the friction coefficient between the water droplet and the solid wall**
Akinori Fukushima, Toshiki Mima, Ikuya Kinefuchi, Takashi Tokmasu

1P27 ☆**Molecular Dynamics Simulation for Melting Process of Various types of Core-Shell Nanoparticles**
Yuki Tamura, Noriyoshi Arai

1P28 **Molecular Simulation Study of Structure and Dynamical Properties of Nitrate Anion in Sodium Chloride Aqueous Solution**
Shigeki Matsunaga

1P29 ☆**Application of a Liquid Theory to Colloidal Dispersion Systems**
Masao Inoue, Akira Yoshimori

1P30 **Dynamic Simulations of Ion Atmosphere of Complex Electrolytes Solutions**
Hitoshi Washizu, Tomoyuki Kinjo, Hiroaki Yoshida

1P31 **A VT Replica Exchange Molecular Dynamics Study in Ultra Supercooled TIP4P/2005 Water**
Liang-Chun Liu, Jer-Lai Kuo

1P32 **Molecular dynamics simulation of vapour-liquid nucleation of water: determining formation energy of a cluster**
Akio Kawano, Kyoko K. Tanaka, Hidekazu Tanaka

1P33 ☆**All-atom Analysis of Electrical Conductivity in Concentrated Electrolyte Solutions**
Kai-Min Tu, Nobuyuki Matubayasi

1P34 ☆**Development of Ab-initio Mean-force Dynamics Using a Logarithmic Energy Landscape for Constructing Free-Energy Profiles**
Makoto Nakamura, Masao Obata, Tetsuya Morishita, Tatsuki Oda

1P35 **Hybrid quantum mechanics (QM) / molecular mechanics (MM) molecular dynamics (MD) simulation of catalytic mechanism by complex of Ras and Ras-GAP: Full description of catalytic mechanisms**
Masaru Tateno, Tetsuhiko Itagaki, Jiyoung Kang

1P36 ☆**A variational path integral molecular dynamics study of molecules using a fourth order propagator**
Yuki Kamibayashi, Shin-ichi Miura

1P37 **Analyses of Coarse-Grained Equation of Motion**
Shiaki Hyodo

1P38 ☆**Molecular Dynamics Simulations of Surfactant Interfaces Using Coarse-Grained Force Field**
Chunwei Yang, Huai Sun

1P39 ☆**Nuclear quantum effect on $OH^-(H_2O)_2$ with *ab initio* path integral molecular dynamics**
Yudai Ogata, Yukio Kawashima, Kaito Takahashi, Masanori Tachikawa

1P40 **A Theory of Phase Transition for Two-Minimum Potential Systems**
Ayumi Suematsu, Akira Yoshimori, Masafumi Saiki, Jun Matsui, Takashi Odagaki

1P41 **A Boundary Condition for Multilevel Simulations for Diffusive Systems**
Motoyuki Shiga, Marco Masia

1P42 **Direct Formation of "Janus"-Particles via Molecular Dynamics Simulations**
Jan-Hubert Antonio Wittmann, Reinhard Strey

1P43 ☆**Molecular Dynamics Simulation on Complexation of a Charged Dendrimer with a Linear Polyelectrolyte**
Satoshi Isono, Akira Kazuno, Susumu Fujiwara, Takashi Itoh, Masato Hashimoto

1P44 **Molecular dynamics simulation for shape change of water-in-oil droplets**
Naohito Urakami, Akio Takaki, Masayuki Imai, Takashi Yamamoto

1P45 ☆**Gelation of tetrahedral monomers studied by molecular dynamics simulation**
Shizuka Ogawa, Takeshi Miyakawa, Ryota Morikawa, Masako Takasu, Takamasa Sakai, Ung-il Chung

1P46 **Monte Carlo Simulations of Structure and Entanglements in Polymer Melts**
Krzysztof Moorthi, Kazunori Kamio, Javier Ramos, Doros N Theodorou

1P47 **Band Gap Design of Thiophene Polymer Based on The Density Functional Theory**
Patricia Lubis, Mineo Saito

1P48 **A numerical simulation of Brownian-particle suspensions using the lattice Boltzmann method**
Hiroaki Yoshida, Tomoyuki Kinjo, Hitoshi Washizu

1P49 **Structural Analysis of Telechelic Polymer Solutions -A Dissipative Particle Dynamics Study-**
Noriyoshi Arai

1P50 **Tetratic phase of bilayer systems under geometrical confinement: Monte Carlo simulation**
Takamichi Terao

1P51 ☆**Thermal conductivity in binary and ternary mixed system of molten alkali halides**
Yoshiki Ishii, Keisuke Sato, Norikazu Ohtori, Mathieu Salanne, Paul Anthony Madden

1P52 ☆**The dependence of ordering process on Coulombic interaction treatment 5CB system**
Takuma Nozawa, Kazuaki Takahashi, Tetsu Narumi, Kenji Yasuoka

1P53 **First principles calculation of the PCBM on the TiO_2 anatase (001) surface**
Kiyotaka Fujino, Mineo Saito

1P54 **Molecular Photovoltaic Devices and Density-functional Theory Simulation**
Shozo Yanagida, Kazuhiro Manseki

1P55 **First-Principles Calculation of Surface State in Topological Insulators Bi_2Te_3 and Related Materials: Film Thickness Dependence**
Takehiro Kato, Hiroki Kotaka, Fumiyuki Ishii

1P56 ☆**Nitrogen Adsorption and Dissociation on Double-Icosahedral Ru_{19} nanocluster - A First-Principle Investigation**
Chen-Hao Yeh, Jia-Jen Ho

1P57 **The Highly Effective Catalytic Behavior of a Metal Nanocluster Ru_{79} on the Dissociation of a N_2 Molecule - A Quantum-chemical Calculation**
Shiuan-Yau Wu, Chen-Hao Yeh, Jia-Jen Ho

1P58 **Magnetic Dipole-Dipole Interaction and Magnetic Structure in Solid Oxygen**
Dewi Muliyati, Masao Obata, Makoto Nakamura, Suprijadi Haryono, Tatsuki Oda

Poster day 2

2P01 ☆**Study of Water-Methanol Mixture Flowing into Carbon Nanotubes with Molecular Dynamics Simulation: Effect of Electric Field**
Winarto, Daisuke Takaiwa, Eiji Yamamoto, Takuma Akimoto, Kenji Yasuoka

2P02 ☆**Study of aqueous NaOH solution surface via computational analysis of sum frequency spectra**
Takako Imamura, Tatsuya Ishiyama, Akihiro Morita

2P03 **Quantum simulation for exotic molecules: Quantum Monte Carlo and Path Integral approach**
Katsuhiko Koyanagi, Yukiumi Kita, Kenta Yamada, Yukio Kawashima, Masanori Tachikawa

2P04 **Vibrational Spectroscopic Response at Water/Vapor and Ice/Vapor Interfaces : Effect of Charge Transfer**
Tatsuya Ishiyama, Hideaki Takahashi, Akihiro Morita

2P05 ☆**Solubility of hydrophobic molecules at the liquid-vapor interfaces of water and simple liquids**
Kiharu Abe, Kenichiro Koga

2P06 **Free energy analysis of CO_2 dissolved in room temperature ionic liquids**
Ryosuke Ishizuka, Nobuyuki Matubayasi

2P07 ☆**Pore Formation Dynamics in Phospholipid/Cholesterol Bilayer under Stretching: System Size Dependence**
Taiki Shigematsu, Kenichiro Koshiyama, Shigeo Wada

2P08 **System size dependence of vapor/liquid coexistence of water in hydrophobic nanocylinder**
Toshiki Mima, Ikuya Kinefuchi, Akinori Fukushima, Takashi Tokumasu, Shu Takagi, Yoichiro Matsumoto

2P09 **Molecular Dynamics Simulation of L-J Fluids near a Heating Surface**
Kazuhiro Itoh, Hiroshige Kumamaru, Yuji Shimogonya

2P10 **The observation of the longitudinal wave velocity in a model supercooled liquid**
Tadashi Muranaka, Jun Matsui, Yasuaki Hiwatari

2P11 **Distance Constraint Networks in Glass-Forming Liquids**
Yasushi Takeuchi

2P12 **Hydrophobic Cavity in the Potassium Channels: Anomalous Nanospace Controlling Ion Conduction**
Takashi Sumikama, Shinji Saito, Shigetoshi Oiki

2P13 **Diffusion of Ions in the Salt Solutions between Ice Walls**
Yuta Nohara, Yoshimichi Hagiwara

2P14 **Glass Transition in One-Component Soft-Core System**
Junko Habasaki, Akira Ueda

2P15 ☆**Guest-host hydrogen bond in sII and sH amyl-alcohol hydrate from molecular dynamics simulation**
Masaki Hiratsuka, Ryo Ohmura, Amadeu K Sum, Kenji Yasuoka

2P16 **A new scaling relation for nucleation rates**
Kyoko K. Tanaka, Hidekazu Tanaka, Juerg Diemand, Raymond Angelil

2P17 **Relaxation Mode Analysis for Biomolecules**
Ayori Mitsutake, Yuta Koizumi, Toshiki Nagai, Hiroshi Takano

2P18 **Evaluation of Protein-Protein Complex Model Using Molecular Dynamics Simulation with the Solution Theory in the Energy Representation**
Kazuhiro Takemura, Nobuyuki Matubayasi, Akio Kitao

2P19 **Free energy calculation of protein conformational changes using parallel cascade selection molecular dynamics simulation and Markov state model**
Yasutaka Nishihara, Ryuhei Harada, Akio Kitao

2P20 **Free energy analysis of flip-flop motion of protein in phospholipid bilayer**
Tomoko Mizuguchi, Nobuyuki Matubayasi

2P21 **Hybrid QM/MM simulation of bovine cytochrome *c* oxidase (I) : Double-stratified architecture for electron transfer**
Jiyoung Kang, Masaru Tateno

2P22 **The Interaction Between Transmembrane Region of Amyloid Precursor Protein (APP) and Cholesterols.**
Naoyuki Miyashita, Fumiko Ogushi, Yuji Sugita

2P23 **Difficulty of Observation of Attractive Part in Effective Interaction between Like-Charged Proteins: a Theoretical Study with Simple Models**
Ryo Akiyama, Takumi Yamashita

2P24 **A Molecular Dynamics Study on the Antigen-Antibody Interactions**
Takefumi Yamashita, Hideaki Fujitani

2P25 **A model-potential-free analysis of protein-protein interactions using small-angle X-ray scattering**
Tomonari Sumi, Hiroshi Imamura, Takeshi Morita, Yasuhiro Isogai, Keiko Nishikawa

2P26 **Computational study of protein-ligand interactions: Molecular screening for therapeutic drugs**
Yosinori Hirano, Noriaki Okimoto, Makoto Taiji

2P27 ☆**Theoretical Study for Understanding the Mechanism of Amyloid Fibril Formations**
Naohiro Nishikawa, Phuong Nguyen, Philippe Derreumaux, Yuko Okamoto

2P28 **Large-scale and All-atom Molecular Dynamics Simulation of Viruses using the K-computer 2. Development of a Highly Parallelized General-Purpose Molecular Dynamics Simulation Program, MODYLAS**
Yoshimichi Andoh, Noriyuki Yoshii, Kazushi Fujimoto, Keisuke Mizutani, Hidekazu Kojima, Atsushi Yamada, Susumu Okazaki, Kazutomo Kawaguchi, Hidemi Nagao, Kensuke Iwahashi, Fumiyasu Mizutani, Kazuo Minami

2P29 ☆**Large-scale and all-atom molecular dynamics simulation of viruses using the K-computer. 3. Equilibration of the system and the stable structure of poliovirus capsid in solution**
Hidekazu Kojima, Noriyuki Yoshii, Atsushi Yamada, Yoshimichi Andoh, Kazushi Fujimoto, Keisuke Mizutani, Atsushi Nakagawa, Akio Nomoto, Susumu Okazaki

2P30 ☆**Inhomogeneous dielectric environment of F_o motor using dipole-dipole correlation**
Asahi Konno, Koji Umezawa, Mitsunori Takano

2P31 **The elucidation of the phase transition mechanism for biomechanical material application of Ti-Ni-Cu alloy**
Shuichi Ikeda, Shiaki Hyodo

2P32 ☆**MD simulations of ATP/ADP bound form of Ca^{2+}-ATPase using improved polyphosphate parameters of the CHARMM force field**
Yasuaki Komuro, Suyong Re, Chigusa Kobayashi, Eiro Muneyuki, Yuji Sugita

2P33 **New generalized ensemble algorithm without the detailed balance condition**
Satoru G. Itoh, Hisashi Okumura

2P34 ☆**Analysis of the structural transition of a chignolin molecule using the 3D-RISM/MD hybrid simulation method**
Shinnosuke Gyoubu, Shinichi Miura

2P35 **An efficiently extendable and fine-grain parallelized molecular dynamics simulation program: Mid**
Takahiro Koishi, Hironori Takeich

2P36 **A simulation method for protein systems by replica-exchange molecular dynamics using genetic crossover**
Yoshitake Sakae, Tomoyuki Hiroyasu, Mitsunori Miki, Katsuya Ishii, Yuko Okamoto

2P37 **A 3D-RISM integral equation study of hydrated peptides**
Hiroshi Iwasaki, Shinichi Miura

2P38 **Generalized centroid molecular dynamics**
Atsushi Horikoshi

2P39 ☆**Theoretical studies of redox potential for metalloprotein by combining MD and QM/MM simulations**
Masashi Iwayama, Hiroaki Saito, Kimikazu Sugimori, Kazutomo Kawaguchi, Hidemi Nagao

2P40 ☆**Development of a Simultaneous Simulation Method for Phonons and Electrons**
Yusuke Masao, Honami Imanishi, Mitsuhiro Matsumoto

2P41 ☆**Spontaneous self-assembly of diblock copolymers in nanoconfined geometries by dissipative particle dynamics**
Koji Takahashi, Takahiro Koishi

2P42 **Bottom-up construction of interaction models of non-Markovian dissipative particle dynamics**
Yuta Yoshimoto, Ikuya Kinefuchi, Toshiki Mima, Akinori Fukushima, Takashi Tokumasu, Shu Takagi

2P43 **Multiscale simulation for thermo-hydrodynamic lubrication of a polymeric liquid between parallel plates**
Shugo Yasuda, Ryoichi Yamamoto

2P44 **Molecular Dynamics Simulation Study on the High Pressure Behavior of a Peptide**
Yoshiharu Mori, Hisashi Okumura

2P45 ☆**Heterogeneous Dynamics of Supercooled Polymer Melts: Relaxation Mode Analysis Study**
Nobuyuki Iwaoka, Hiroshi Takano

2P46 **Thermal Statibilty of Gramicidin A in Lipid Bilayer: A Molecular Dynamics Study**
Hiroaki Saito, Kawaguchi Kazutomo, Hidemi Nagao

2P47 **Coarse-grained Molecular Simulation for Viscoelastic Properties of Polyurethane Shape Memory Polymer**
Shimpei Matsuda, Masaaki Nishikawa, Masaki Hojo

2P48 **Interaction of the nucleotide with a phospholipid bilayer: a molecular dynamics simulation study**
Daisuke Takaiwa, Kenji Yasuoka, Toshikazu Ebisuzaki

2P49 **Relaxation modulus connection between Atomistic and Coarse-Grained Molecular Simulation of Polymer Melts using the Rouse Parameters**
Nobuyoshi Yamato, Iori Yonekawa, Kazuaki Z Takahashi, Kenji Yasuoka, Yuichi Masubuchi

2P50 ☆**Phase Transition between Ice VII and Plastic Ice**
Kazuhiro Himoto, Masakazu Matsumoto, Hideki Tanaka

2P51 **First-Principles Study of Artificial Superlattice $(LaMnO_3)_n/(SrTiO_3)_m$**
Miho Nishida, Fumiyuki Ishii, Hiroki Kotaka, Mineo Saito

2P52 **Uncovering a Dynamically Formed Substrate Access Tunnel in Carbon Monoxide Dehydrogenase/Acetyl-CoA Synthase**
Po-hung Wang, Maurizio Bruschi, Luca De Gioia, Jochen Blumberger

2P53 ☆**Reactive Force Field (ReaxFF) Developed for Aluminophosphate Zeolite**
Liang Xin, Huai Sun

2P54 **Magnetism and electronic structure calculations of Pd-TM alloys and hydrogen system**
Norio Nunomura, Masanori Hara, Satoshi Akamaru

2P55 **Analysis for Crystal Growth of Methane Hydrate from Molecular Dynamics Simulation**
Daisuke Yuhara, Daisuke Takaiwa, Kenji Yasuoka

2P56 **Comparative ab initio Calculation Studies of Hydration Structures on Cs and other Alkaline metals**
Masahiko Machida, Kazuhiro Sakuramoto, Masahiko Okumura, Hiroki Nakamura, Yuya Sato, Keiko Akutsu, Motoyuki Shiga

2P57 ☆**Molecular Dynamics Study on Carbon Diffusion Mechanism of Pearlitic Steel in Wiredrawing**
Yohei Sameshima, Ken-ichi Saitoh, Masanori Takuma, Yoshimasa Takahashi

2P58 ☆**DFT Study of Negatively Charged Oxygen Vacancy on (110) TiO_2 Surface**
Taizo Shibuya, Kenji Yasuoka, Susanne MIrbt, Biplab Sanyal

2P59 **Evidence of Phonon-Assisted Auger Recombination and Multiple Exciton Generation in Semiconductor Quantum Dots Revealed by Temperature-Dependent Phonon Dynamics**
Hyeon-Deuk Kim

Poster day 3

3P01 ☆**Dual effect of crowders on fibrillation kinetics of polypeptide chains revealed by lattice models**
Nguyen Truong Co, Chin-Kun Hu, Mai Suan Li

3P02 ☆**A Molecular Simulation Study to Investigate Actin Filament Elongation Mechanism**
Nobuhiko Wakai, Yasutaka Nishihara, Kazuhiro Takemura, Takashi Fujii, Keiichi Namba, Akio Kitao

3P03 ☆**Replica exchange MD and *ab initio* fragment MO calculations on effects of solvating water molecules on stable conformations of amyloid-β dimer**
Akisumi Okamoto, Atsushi Yano, Kazuya Nomura, Shin'ichi Higai, Noriyuki Kurita

3P04 **MHC I Recognition Mechanism of MIR2 from Kaposi's Sarcoma-Associated Herpesvirus**
Pai-Chi Li, Mizuho Kajikawa, Naoyuki Miyashita, Satoshi Ishido, Yuji Sugita

3P05 **Multiple molecular dynamics simulations of human adult haemoglobin: Novel intra-molecular signal propagation pathways for nonlinear response in ligand-binding**
Tetsuhiko Itagaki, Jiyoung Kang, Masaru Tateno

3P06 **Hybrid QM/MM simulation of bovine cytochrome *c* oxidase (II): Dynamical mechanisms of ligand recognition**
Toru Matsuoka, Jiyoung Kang, Masaru Tateno

3P07 **Standard free energy of binding for theophylline and caffeine to RNA aptamer using alchemical transformation**
Yoshiaki Tanida, Azuma Matsuura

3P08 **Theoretical Prediction for Crystal Structures of Semiconducting and Pharmaceutical Organic Molecules**
Shigeaki Obata, Yukihiro Shimoi, Toshiaki Miura, Hitoshi Goto

3P09 **Effect of surface-bound protein aggregates on the structure the host membran: A CGMD study with 3D stress field analysis**
Hualin Li, Alemayehu Gorfe

3P10 **Molecular dynamics study on mean force between Hsp90 and ADP**
Kazutomo Kawaguchi, Hiroaki Saito, Hidemi Nagao

3P11 **Large-scale and all-atom molecular dynamics simulation of viruses using the K-computer: 4. Negative pressure inside the poliovirus empty capsid**
Kazushi Fujimoto, Yoshimichi Andoh, Noriyuki Yoshii, Atsushi Yamada, Hidekazu Kojima, Keisuke Mizutani, Atsushi Nakagawa, Akio Nomoto, Susumu Okazaki

3P12 **All-Atom Modelling and Molecular Dynamics Simulation of the Cytoplasm of Mycoplasma Genetalium**
Isseki Yu, Takaharu Mori, Jaewoon Jung, Ryuhei Harada, Yuji Sugita, Michael Feig

3P13 **Large-Scale and All-Atom Molecular Dynamics Simulation of Viruses using the K-computer: 5. Molecular Designs for a Stable Viral Capsid**
Noriyuki Yoshii, Yoshimichi Andoh, Atsushi Yamada, Kazushi Fujimoto, Hidekazu Kojima, Keisuke Mizutani, Atsushi Nakagawa, Akio Nomoto, Susumu Okazaki

3P14 **Large-scale and all-atom molecular dynamics simulation of viruses using the K-computer : 6. Exchange of water molecules across the poliovirus capsid**
Atsushi Yamada, Noriyuki Yoshii, Yoshimichi Andoh, Kazushi Fujimoto, Hidekazu Kojima, Keisuke Mizutani, Atsushi Nakagawa, Akio Nomoto, Susumu Okazaki

3P15 **First-Principles Study of Organic Molecular Antiferroelectric Squaric Acid**
Fumiyuki Ishii, Yoshiki Tanaka

3P16 **Conformational change of SERCA upon alternating protonation states in Ca^{2+}-binding site**
Chigusa Kobayashi, Yuji Sugita

3P17 **Collective Motion in Super Ionic Conductive Glasses**
Teruyoshi Awano

3P18 ☆**Large-Scale MD Simulation of Quasi Liquid Layer of Ice with Dislocation**
Yasuhiro Kajima, Shuji Ogata, Ryo Kobayashi, Tomoyuki Tamura, Yohei Niwa

3P19 **Mapping of dissipative particle dynamics model onto vapor-liquid coexistence**
Tomoyuki Kinjo, Hiroaki Yoshida, Hitoshi Washizu

3P20 **Response of Thin Liquid Film to Microscale Projectiles**
Toshihiro Nakatani, Mitsuhiro Matsumoto

3P21 **Transverse and longitudinal modes in liquids from molecular-dynamics simulations**
Shuji Munejiri, Kozo Hoshino

3P22 **Dissipative Particle Dynamics Simulation of Nanometer-Thick Liquid Lubricant Films under Shear**
Motoo Fukuda, Hedong Zhang, Hitoshi Washizu, Tomoyuki Kinjo, Hiroaki Yoshida, Kenji Fukuzawa, Shintaro Itoh

3P23 ☆**Analysis of Ion Transport by Using 2D Free Energy Profile**
Nobuaki Kikkawa, Akihiro Morita

3P24 ☆**Large-Scale and All-Atom Molecular Dynamics Simulation of Viruses Using the K-computer: 7. Interaction with Poliovirus Receptor CD155**
Keisuke Mizutani, Noriyuki Yoshii, Atsushi Yamada, Yoshimichi Andoh, Kazushi Fujimoto, Hidekazu Kojima, Atsushi Nakagawa, Akio Nomoto, Susumu Okazaki

3P25 ☆**The concentration and halide ion effect of the ionic cluster**
Katsufumi Tomobe, Eiji Yamamoto, Kojic Dusan, Masato Yasui, Kenji Yasuoka

3P26 **Water monolayer: a simple model of hydrophilic wall**
Lukman Hakim, Masakazu Matsumoto, Hideki Tanaka

3P27 ☆**Molecular Dynamics Simulation on Conformational Fluctuation and Water Transport within AQP1**
Eiji Yamamoto, Takuma Akimoto, Yoshinori Hirano, Masato Yasui, Kenji Yasuoka

3P28 **Thermodynamics and Molecular Dynamic Simulations of Three-phase Equilibrium in Argon (v6)**
Yosuke Kataoka, Yuri Yamada

3P29 ☆**Microstructure Analysis of Sedimenting Particles**
Adnan Hamid, John Jairo Molina, Ryoichi Yamamoto

3P30 **Simulation of metal-ligand self-assembly into spherical complex**
Makoto Yoneya, Tomohiko Yamaguchi, Sota Sato, Makoto Fujita

3P31 ☆**Gel-fluid phase transitions in asymmetric lipid bilayers**
Antti Lamberg, Takashi Taniguchi

3P32 **Anomalous water dynamics on the membrane surface**
Takuma Akimoto, Eiji Yamamoto, Masato Yasui, Kenji Yasuoka

3P33 **Prediction of Structure and Dynamics of Glycans from Molecular Dynamics Simulations**
Suyong Re, Wataru Nishima, Shigehisa Watabe, Yuji Sugita

3P34 **A molecular dynamics study on the viscoelasticity of cross-linked polymers**
Yuji Kataoka, Hiroyuki Takahashi, Osamu Hino

3P35 ☆**Diffusion mechanism of CO_2 in a crystalline polymer membrane studied using model gases**
Shunsuke Asahi, Yoshinori Tamai

3P36 **Molecular Dynamics Study on Nanoconfined Liquid Crystal**
Hiroki Matsubara, Fabio Pichierri, Kazue Kurihara

3P37 ☆**A Molecular Dynamics Study of Free Energy Profile of a Pair of Aggregates in the Formation Process of SDS Micelle**
Shinji Kawada, Kazushi Fujimoto, Noriyuki Yoshii, Susumu Okazaki

3P38 ☆**Molecular Dynamics Study of Free Energy Profile of Solubilization of Insoluble Molecules in Ionic SDS and Non-ionic $C_{12}E_8$ Micelles**
Hiroaki Takabayashi, kazushi Fujimoto, Noriyuki Yoshii, Susumu Okazaki

3P39 **Tribology of Polymer Brush: Microscale Modeling and Simulation**
Mitsuho Ide, Mitsuhiro Matsumoto

3P40 **First-principles electronic structure calculations of the wurtzite ZnO slab**
Van-Minh Vo, Makoto Nakamura, Masao Obata, Mineo Saito, Fumiyuki Ishii, Tatsuki Oda

3P41 **Ab initio study of electric polarization and spin textures in ATiO$_3$ (A=Pb, Ba) with structural phase transition**
Takashi Onishi, Fumiyuki Ishii, Hiroki Kotaka, Mineo Saito

3P42 ☆**Theoretical analysis of dynamic feature for self-assembled nanocube in aqueous solution**
Takako Mashiko, Shuichi Hiraoka, Umpei Nagashima, Masanori Tachikawa

3P43 ☆**Density-functional Calculations on the Adsorption and Dissociation of Nitric oxide on Rh and Ni Nanoclusters**
Chun-Chih Chang, Jia-Jen Ho

3P44 ☆**Density-functional Calculations of Methanol Sythesis from Methane Oxidation on Pt_2-Graphene Oxide Surface**
Chien-Hao Lin, Jia-Jen Ho

3P45 **Heterogeneous Nucleation on Various Seed Configurations by Molecular Dynamics**
Donguk Suh, Kenji Yasuoka

3P46 **Microscopic Mechanism of Cs Strong Affinity on Clay Minerals through ab initio Calculations**
Masahiko Okumura, Hiroki Nakamura, Masahiko Machida

3P47 ☆**A study for homogeneous melting dynamics of a high pressure polymorph of ice: ice VI**
Kenji Mochizuki, Masakazu Matsumoto, Iwao Ohmine

3P48 **DOS Estimation for the Soft Core System**
Hisashi Shimizu

3P49 **Optimized vibrational coordinates for anharmonic vibrational structure theories**
Kiyoshi Yagi, Murat Keçeli, So Hirata

3P50 **Sequential data assimilation to single-molecule FRET photon-counting data by using molecular dynamics simulations**
Yasuhiro Matsunaga, Yuji Sugita

3P51 **Midpoint cell method for hybrid (MPI+OPENMP) parallelization of Molecular Dynamics**
Jaewoon Jung, Takaharu Mori, Yuji Sugita

3P52 **Vibrational Quasi-degenerate Perturbation Theory with Optimized Vibrational Coordinates: Applications to Ethylene and 1,3-Butadiene**
Hiroki Otaki, Kiyoshi Yagi

3P53 **Multi-scale Sampling using Temperature Accelerated and Replica exchange Molecular Dynamics**
Yu Yamamori, Akio Kitao

3P54 **Applications of a Linear-combination-based Isotropic Periodic Sum Method in Molecular Dynamics Simulations**
Kazuaki Z. Takahashi, Takuma Nozawa, Shun Kameoka, Tetsu Narumi, Donguk Suh, Kenji Yasuoka

3P55 ☆**Control of the Automated Guided Vehicle System via Molecular Dynamics Algorithm**
Ko Ohashi, Shiaki Hyodo

3P56 ☆**GPU Accelerated Replica Exchange Molecular Dynamics Simulation of Lennard-Jones Fluid**
Kentaro Nomura, Minoru Oikawa, Atsushi Kawai, Tetsu Narumi, Kenji Yasuoka

3P57 **Modeling of Energy Transport in Solid Based on Boltzmann Transport Equations**
Hirofumi Kurata, Honami Imanishi, Yusuke Masao, Mitsuhiro Matsumoto

3P58 **Multiscale Simulation of Entangled Polymer Melt with Elastic Deformation**
Takahiro Murashima