

## **JST International Symposium on Multi-scale Simulation of Condensed-phase Reacting Systems**

### **Poster List**

- P01** Theoretical Study of Absorption and Fluorescence Spectra of Firefly-Luciferin

*Miyabi Hiyama, Hidefumi Akiyama, Kenta Yamada, Nobuaki Koga*

- P02** Two-layer QM/QM' Calculations for Binuclear Active Site

*Y. Kitagawa, N. Yasuda, H. Hatake, T. Matsui, T. Kawakami, S. Yamanaka,  
M. Okumura, K. Yamaguchi*

- P03** Conformational Change of U1A Protein: Molecular Dynamics Simulation Study

*Ikuo Kurisaki, Masayoshi Takayanagi, Masataka Nagaoka*

- P04** ATP Hydrolysis Free Energy Barriers in Kinesin

*Matthew J. McGrath, I.-Feng William Kuo, Shoji Takada*

- P05** Protein Denaturation by Heat and Pressure Studied by Multibaric-multithermal

Molecular Dynamics Simulation

*Hisashi Okumura*

- P06** Ligand-protein Interaction Studied by Computer Simulation and Time-resolved X-ray

Crystallography

*T. Tsuduki, A. Tomita, S. Koshihara, S. Adachi, T. Yamato*

- P07** Molecular Dynamics Study on the Enzymatic Mechanism of Limonen Epoxide

Hydrolase

*Yasushige Yonezawa*

- P08** On the Smoothing of Free Energy Landscape of Neutral-Form Glycine Conformers in Aqueous Solution  
*Yukichi Kitamura, Norio Takenaka, Yoshiyuki Koyano, Masataka Nagaoka*
- P09** Enhanced Thermal Diffusion of Li in Graphite by Alternating Vertical Electric Field: A Hybrid Quantum-Classical Simulation Study  
*Nobuko Ohba, Shuji Ogata, Tomoyuki Tamura, Ryo Kobayashi, Shunsuke Yamakawa, Ryoji Asahi*
- P10** Addition and Abstraction Reactions of OH with Benzoate Anion  
*Nobuaki Tanaka, Hiromasa Nishikiori*
- P11** Analysis of Entropic Effect on the Lattice Defect Migration by Using Free Energy Gradient Method  
*Hideki Mori*
- P12** IR Stealth Effect for Molecules Adsorbed on Single-Walled Carbon Nanotubes  
*Yoshifumi Nishimura, Dmitry V. Kazachkin, Henryk A. Witek, Eric Borguet, Stephan Irle*
- P13** Computational Chemical Analysis of the Nanostructures of the Macromolecular Polymer Membranes  
*Yuichi Suzuki, Yoshiyuki Koyano, Takuya Okamoto, Masataka Nagaoka*
- P14** Molecular and Electronic Structures of the Super Reduced State of a Polyoxometalate (POM),  $[Mo_{12}O_{40}P]^x$  ( $x = -3, -27$ )  
*Yoshio Nishimoto, Hirofumi Yoshikawa, Kunio Awaga, Stephan Irle*
- P15** Measurement of Kinetic Energies of Fragments Produced by the Photodissociation of  $C_{70}$  Using Velocity Map Imaging  
*Hideki Katayanagi, Koichiro Mitsuke*
- P16** Theoretical Study of Electron Transfer Reaction by Photolyase/Cryptochrome Blue-Light Photoreceptors  
*Ryuma Sato, Takahisa Yamato*

- P17** Density Functional Study of NO-selectivity of Co-center in N<sub>2</sub>S<sub>2</sub> coordination environment  
*Hiroaki Wasada, Yuko Wasada-Tsutsui, Zhang Zizheng, Tomohiro Hashimoto, Takuma Yano, Tomohiko Inomata, Yasuhiro Funahashi, Tomohiro Ozawa, Hideki Masuda*
- P18** Exploring Free Energy Landscape for Chemical Reaction: Routes of Fenton's Reagent to Oxidizing Agents  
*Norifumi Yamamoto, Nobuaki Koga*
- P19** Theoretical Studies on 1,3-Hydrogen Transfer Reaction of Allylamines Catalyzed by Rh(I)-BINAP  
*Takayoshi Yoshimura, Yoshiyuki Kenmotsu, Satoshi Maeda, Keiji Morokuma, Seiji Mori*
- P20** A Dual-Genetic Algorithm Approach to Determine Lowest Energy Isomers of Functionalised Fullerenes  
*Matthew A. Addicoat, Alister J. Page, Keiji Morokuma, Stephan Irle*
- P21** Quantum Chemical Study of Ultraviolet Bonding of Perfluoropolyethers to Graphene  
*Md. Khorshed Alam, Hedong Zhang*
- P22** Electron Wave Packet Modeling of Chemical Bonding  
*Koji Ando*
- P23** Path Search and Path Sampling Algorithms for Complex Molecular Systems  
*Hiroshi Fujisaki, Motoyuki Shiga, Akinori Kidera*
- P24** Atomic Stress Tensor Analysis of Biomolecules  
*Takakazu Ishikura, Tatsurou Hatano, Takahisa Yamato*
- P25** Fragment Molecular Orbital Study on Electron Tunneling Mechanism of Electron Transfer Reaction from Heme c-559 to Photo-oxidized Special Pair P960<sup>+</sup> in Bacterial Photosynthetic Reaction Center  
*Hirotaka Kitoh-Nishioka, Koji Ando*

- P26** Concurrent Coupling of Atomistic and Coarse-Grained Methods for Solid  
*Ryo Kobayashi, Shuji Ogata*
- P27** Development of Protein Force Field Using a Modified Backbone-torsion-energy Term  
*Yoshitake Sakae, Yuko Okamoto*
- P28** Development of Isotropic Site-site Potential for Exchange Repulsion Energy Based on Ab Initio Calculation  
*Daisuke Yokogawa, Stephan Irle*
- P29** Multi-hierarchy Molecular Dynamics with Affine Coupling Method  
*Atsushi M. Ito, Hisashi Okumura, Arimichi Takayama, Hiroaki Nakamura*
- P30** Application of Replica-Exchange Molecular Dynamics to Lipid Bilayer Systems with a Coarse-Grained Model  
*Tetsuro Nagai, Yuko Okamoto*
- P31** Proton Transfer Reaction of Malonaldehyde Studied by *Ab Initio* Generalized-Ensemble Molecular Dynamics Simulations  
*Yoshiharu Mori, Yuko Okamoto*
- P32** Implementation of AMBER-PAICS Interface  
*Takuya Okamoto, Takeshi Ishikawa, Yoshiyuki Koyano, Norifumi Yamamoto, Kazuo Kuwata, Masataka Nagaoka*
- P33** A Mixed Quantum-Classical Molecular Dynamics Study of Intramolecular Proton Transfer Reaction of Malonaldehyde in Non-Polar and Protic Polar Solvent  
*Hidekazu Kojima, Atsushi Yamada, Susumu Okazaki*
- P34** Visualization of the Protein Transfer Free Energy: Toward the Microscopic Understanding of the Molecular Crowding Effect  
*Isseki Yu, Kyoko Nakada, Masataka Nagaoka*

- P35** Primary Events of Photodynamics of All-trans Retinal Protonated Schiff Base in Bacteriorhodopsin, Methanol Solution and Gas Phase  
*Xin Li, Lung Wa Chung, Keiji Morokuma*

- P36** DFT Studies of the Structural Variety of the Cu<sub>2</sub>S<sub>2</sub> Core of the Cu<sub>A</sub> Site  
*Yu Takano, Orio Okuyama, Yasuteru Shigeta, Haruki Nakamura*

- P37** QM/MM CPMD Study on the Acylation of Nylon Oligomer Hydrolase  
*Takeshi Baba, Katsumasa Kamiya, Toru Matsui, Mauro Boero, Seiji Negoro, Yasuteru Shigeta*

- P38** Computer Aided-molecular Design to Optimal Drug Design: Applications to Anti-TB Agents, Anti-cancer Agents and Anti-HIV-1 Inhibitors  
*Pornpan Pungpo, Auradee Punkvang, Parit Khumsri, Dararat Kasamsri, Apinya Srisupan, Patchreenart Saparpakorn, Supa Hannongbua, Peter Wolschann, Supakit Prueksaaroon*