

## Poster Session

- P1: Aditi Guputa, Bundet Boekfa, Hidehiro Sakurai, Masahiro Ehara, and U. Deva Priyakumara  
Structure, Interaction and Dynamics of Au/Pd Bimetallic Nanoalloys Dispersed in Polyvinylpyrrolidone (PVP)
- P2: Yuki Kanazawa, Masahiro Ehara, and Thomas Sommerfeld  
Low-lying  $\pi^*$  Resonances of Standard and Rare DNA and RNA Bases Studied by the Projected CAP/SAC-CI Method
- P3: Pedro J. Castro and Keiji Morokuma  
Quantum chemistry study on the electroluminescence of some Organic-LEDs (OLEDs)
- P4: Maneeporn Puripat, Romain Ramozzi, Miho Hatanaka, Waraporn Parasuk, Vudhichai Parasuk, and Keiji Morokuma  
The Biginelli reaction is a urea-catalyzed organocatalytic multicomponent reaction
- P5: Takafumi Shiraogawa, Ryoichi Fukuda, and Masahiro Ehara  
Theoretical Study on Circular Dichroism and Circularly Polarized Luminescence of Metal Complexes
- P6: Yasuhiro Shigemitsu and Yasushi Ohga  
Metadynamics Calculations on Nonequilibrium Coupling of Chemical Reaction and Solvation Fluctuation: Z/E Isomerization as a Case Study
- P7: Ren Xuefeng and Keiji Morokuma  
The Effect of Intramolecular Hydrogen Bonding on the Mechanism of Excited State Decay of Iridium(III) Cyclometalated Complexes
- P8: Carlos Bistafa, Yukichi Kitamura, Masataka Nagaoka, and Sylvio Canuto  
The electronic transitions of paranitrophenol and paranitrophenolate in gas and water: A study combining ab initio multiconfigurational calculations and the free energy gradient method

- P9: Tomoya Ichino, Satoshi Maeda, and Tetsuya Taketsugu  
A computational study on structures and reactivity of  $[\text{Rh}_6(\text{NO})_n]^{q+}$  ( $n = 0-7$ )  
( $q = 0, 1$ ) by artificial force induced reaction method
- P10: Takahide Matsuoka and Kazuo Takatsuka  
Effect of Nonadiabatic Interactions in Ionization Process of Multi-Electron  
Polyatomic Molecule
- P11: Takanori Nagami, Soichi Ito, Takashi Kubo, and Masayoshi Nakano  
Theoretical Study on the Effect of Intermolecular Packing on Singlet Fission in  
Terrylene Dimer
- P12: Hiromasa Tanaka, Yoshiaki Nishibayashi, and Kazunari Yoshizawa  
Theoretical Study on Nitrogen Fixation Catalyzed by Dinitrogen-Bridged  
Dimolybdenum Complexes Bearing PCP-Type Pincer Ligands
- P13: Kazunari Yoshizawa, Hiroyuki Murata, Chisa Higuchi, Takayuki Semoto, and  
Hiromasa Tanaka  
Molecular Understanding of the Mechanism of Adhesion between Epoxy Resin  
and Metal Surface
- P14: Kaoru Yamazaki, Yasunori Miyazaki, Yu Harabuchi, Tetsuya Taketsugu,  
Satoshi Maeda, Yoshiya Inokuchi, Shin-nosuke Kinoshita, Masataka Sumida,  
Yuuki Onitsuka, Hiroshi Kohguchi, Masahiro Ehara, and Takayuki Ebata  
Multi-step Intersystem Crossing Pathways in Cinnamate-based UV-B  
Sunscreens
- P15: Shota Tsujimoto, Naoki Hayakawa, Kazuya Sadamori, Miho Hatanaka,  
Tomorari Wakabayashi, and Tsukasa Matsuo  
Metal-free P=P bond cleavage by N-heterocyclic carbenes. An experimental and  
computational study
- P16: Ken Sakata, Masahiro Yuki, Kazunari Nakajima, and Yoshiaki Nishibayashi  
Oxidation of Hydrogen Molecule Catalyzed by Thiolate-Bridged Dinuclear  
Ruthenium Complex: A DFT Study

- P17: Kentaro Yamamoto and Kazuo Takatsuka  
Photoinduced Charge Separation Catalyzed by Mn-Oxides onto a Y-Shaped Branching Acceptor Efficiently Preventing Charge Recombination
- P18: Yoshio Nishimoto and Fedorov G. Dmitri  
The Fragment Molecular Orbital Method Combined with Density-Functional Tight-Binding and the Polarizable Continuum Model
- P19: Hiroshi Matsui, Yasutaka Kitagawa, and Masayoshi Nakano  
Second Hyperpolarizability of One-Dimensional  $\pi$ -Conjugated Systems Involving Si=Si Double Bonds
- P20: Takuya Iwakawa, Oda Nozomu, Hiroshi Nakano, and Hirofumi Sato  
Toward a method to calculate quantum rate constants of chemical reactions in solution using Ring Polymer Molecular Dynamics method
- P21: Norio Takenaka, Uppula Purushotham, and Masataka Nagaoka  
On Additive Effect of Solid Electrolyte Interphase (SEI) Film Formation in Sodium-Ion Batteries
- P22: Wataru Ota, Maxim Shishkin, and Hirofumi Sato  
Phase Stability and Band Structure of Alkali Metal-Graphite Intercalation Compounds for Their Application as Negative Electrodes in Secondary Batteries
- P23: Yusuke Matsumi, Hiroshi Nakano, and Hirofumi Sato  
Development of a method to study the electronic structure of a redox species at the electrode interface
- P24: Yukichi Kitamura, Norio Takenaka, and Masataka Nagaoka  
Dual Approach to Vibrational Spectra in Solution: Microscopic Influence of Hydrogen Bonding to the State of Motion of Glycine in Water
- P25: Satoshi Suzuki and Keiji Morokuma  
Aggregation-induced emission of BDAA

- P26: Hong Zheng, Kazuhiko Semb, Yoshiaki Nakao, and Shigeyoshi Sakaki  
Theoretical Study on Characteristic Features of Transmetallation between Pd(II)-Ph and Cu(I)-alkyl Complexes
- P27: Jing Lu and Jingping Zhang  
Rational design on tuning the singlet-triplet energy gap and emission wavelength for thermally activated delayed fluorescent materials: a DFT study
- P28: Jia-Jia Zheng, Shinpei Kusaka, Ryotaro Matsuda, Susumu Kitagawa, and Shigeyoshi Sakaki  
CO<sub>2</sub> Adsorption into Soft Porous Coordination Polymer: A Theoretical Study on the Gate-Opening Mechanism
- P29: Eisuke Kawashima, Mikiya Fujii, and Koichi Yamashita  
Morphological Effect on Performance of Organic Photovoltaics
- P30: Maxim Shishkin and Hirofumi Sato  
Application of DFT+U with Magnetic Exchange Method to the Analysis of Redox and Magnetic Properties of Cathode Materials of Li--and Na--ion Batteries
- P31: Kenichiro Saita, Yu Harabuchi, Tetsuya Taketsugu, and Satoshi Maeda  
Mechanism of the Photochemical Ligand Substitution of Tricarbonyl Re(I) Complex
- P32: Akhilesh kumar Sharma, W. M. C. Sameera, Masaharu Nakamura, and Keiji Morokuma  
Computational Insights on the Mechanism and the Origin of Enantioselectivity in Fe-catalyzed Cross-Coupling Reaction
- P33: Yu Harabuchi, Kenichiro Saita, Satoshi Maeda, and Tetsuya Taketsugu  
Systematic Exploration of Non-radiative Decay Pathways: Application to Photoreactions.

- P34: Yanying Zhao and Keiji Morokuma  
Oxidative Activation of Methane by Laser-ablated Copper Atoms Reaction with O<sub>2</sub>: Matrix Isolation Infrared Spectroscopic and Theoretical Investigation
- P35: Masanori Kaneko, Giacomo Giorgi, and Koichi Yamashita  
Effect of Sr vacancies and substitutionals on the optical absorption and the band position of SrNbO<sub>3</sub>: a DFT analysis
- P36: Miho Isegawa, W. M. C. Sameera, Akhilesh Sharma, Taku Kitanosono, Shū Kobayashi, and Keiji Morokuma  
Enantioselective Copper Catalyzed Boron Conjugate Addition: DFT Study on Mechanistic Difference in Copper(I) and Copper(II) Catalysis
- P37: Shinji Aono and Shigeyoshi Sakaki  
QM/MM study of phenyl(phenyl-isocyanide) Gold(I) complex: Effects of molecular crystal on absorption and emission spectra
- P38: Masayuki Nakagaki and Shigeyoshi Sakaki  
Electronic Structure and Bonding Nature of Trinuclear Cr(II) Complex: Remarkably Small Cr-Cr Bond Order and Large Spin Polarization
- P39: Chiaki Hiraiwa, Tomomi Yasoshima, and Azusa Muraoka  
Intermolecular Interaction between a Fullerene and a Double Concave Buckycatcher
- P40: W. M. C. Sameera and Keiji Morokuma  
Theoretical Studies of Complex Catalytic Reactions Using the AFIR Method
- P41: W. M. C. Sameera, Masaki Yoshida, Atsushi Kobayashi, and Masako Kato  
Computational Modelling of Luminescent Mixed-Valent Platinum Clusters
- P42: Arpita Varadwaj, Pradeep R. Varadwaj, and Koichi Yamashita  
On the Physical Understanding of the Outdoor Environmental Stability of the Zero-Dimensional Lead Halide Perovskite Complexes in Water

- P43: Ayako Kubo, Giacomo Giorgi, and Koichi Yamashita  
Ab-initio Investigations on MgTaO<sub>2</sub>N as a Novel Photocatalyst Material:  
Insights from Anion Ordering, Octahedral-tilting and Crystal Polymorphism
- P44: Nozomi Takagi, Kazuya Ishimura, Masafuyu Matsui, Ryoichi Fukuda,  
Masahiro Ehara, and Shigeyoshi Sakaki  
Core-shell vs. Other Structures in Binary Cu<sub>38-n</sub>M<sub>n</sub> Nanocluster (M = Ru, Rh,  
Pd, Ag, Os, Ir, Pt, and Au; n = 1, 2, and 6): Theoretical Insight into Determining  
Factors
- P45: Pradeep R. Varadwaj, Arpita Varadwaj, and Koichi Yamashita  
Unusually High Cooperativity Revealed in the Chemical Bonding Interactions  
Exploited: Novel Lead Iodide Perovskite Complex System as a Prototype
- P46: Kimichi Suzuki, Satoshi Maeda, and Keiji Morokuma  
Theoretical study on ring opening and closing mechanism of diarylethene  
derivatives
- P47: Masafuyu Matsui and Shigeyoshi Sakaki  
Development of an Embedded Cluster Model Incorporating Electrostatic  
Potential
- P48: Masahiko Taguchi, Cheng Cheng, Chika Higashimura, and Shigehiko Hayashi  
QM/MM approach for Light-activation mechanism of LOV photoreceptor  
protein
- P49: Cheng Cheng, Kamiya Motoshi, Yoshida Norio, and Hayashi Shigehiko  
Theoretical study on molecular mechanism of photo-induced gate opening of  
channelrhodopsin
- P50: Yuki Yamamoto, Lu Fengniu, Takashi Nakanishi, and Shigehiko Hayashi  
Molecular dynamics simulations and theoretical analysis of liquid pyrenes
- P51: Ryo Oyama, Taisuke Hasegawa, and Shigehiko Hayashi  
Theoretical study on molecular mechanism of a light-driven ion transport of

Halorhodopsin

P52: Masahiro Kaneko and Shigehiko Hayashi

Theoretical study on catalysis of HIV-1 protease