List of Poster Presentations

Saturday, September 3 (18:30 - 20:30)

3PP-01 *Qiming Sun (Peking University)*
Exact two-component theory for NMR parameters

3PP-02 *Hiroyuki Nohira (Saitama University)*
Quantization of chemical reaction: the dynamic correlation diagram method free from noncrossing rule

3PP-03 *Boris N. Plakhutin (Russian Academy of Sciences)*
Additional variational condition in the ROHF method ensuring a fulfillment of Koopmans'

3PP-04 *Tatiya Chokbunpiam (Chulalongkorn University)*
The electronic properties of organic dyes porphyrin-thiophene-perylene and its derivatives modified by varying thiophene linker

3PP-05 *Ines Urdaneta (Benemerita Universidad Autonoma de Puebla)*
Franck-Condon factors for diatomic molecules for an arbitrary anharmonic potential

3PP-06 *Matthias Degroote (Ghent University)*
Faddeev random phase approximation for molecules

3PP-07 *Minoru Hoshino (Nissan Chemical Industries, LTD.)*
Development and applications of divide-and-conquer constrained self-consistent field method

3PP-08 *Atsushi Kubo (Kyoto University)*
Gauge function optimization for accurate calculations of magnetic wavefunctions

3PP-09 *Stella Stopkowicz (University of Mainz)*
Relativistic corrections via fourth-order direct perturbation theory

3PP-10 *Lan Cheng (University of Mainz)*
Analytic energy derivatives in relativistic quantum chemistry: Rigorous treatments of both scalar-relativistic and electron-correlation effects

3PP-11 *Masayuki Kawahata (Toyohashi University of Technology)*
Solution of time-dependent Schrodinger equation by quantum walk

3PP-12 *Junji Seino (Waseda University)*
Local unitary transformation in two-component relativistic scheme for large-scale molecular systems

3PP-13 *Vasile Georgescu (Romanian Academy)*
Thermoprogrammed reduction and thermoprogrammed desorption studies of metallic and oxidic catalysts

3PP-14 *Takesi Nagata (Kyoto University)*
Recent development of the analytic gradient in the fragment molecular orbital method

3PP-15 *Yuka Nakamura (Kyushu University)*
A perturbation theory for friction of a large particle immersed in a binary solvent

3PP-16 *Zhendong Li (Peking University)*
Spin-adapted open-shell TDDFT

3PP-17 *Shusuke Yamanaka (Osaka University)*
Assessment of density functional theory for calculations of magnetic interactions of manganese complexes

3PP-18 *Hui-Lung Chen (Chinese Culture University)*
Computational investigation on adsorption and dissociation of NH_3 molecule on Fe(111)

3PP-19 *Ayako Nakata (National Institute for Materials Science)*
Spin-orbit TDDFT calculations with long-range correction

3PP-20 *Yu-ichiro Matsushita (The University of Tokyo)*
Comprehensive study of hybrid functionals applied to structural and electronic properties of semiconductors and insulators

3PP-21 *Hyunjun Ji (KAIST)*
Analytic derivatives of quartic-scaling doubly hybrid XYGJ-OS functional: Theory and

3PP-22 *Yasuhiro Ikabata (Waseda University)*
Implementation and numerical assessment of local response dispersion method

3PP-23 *Hossein Tavakol (University of Zabol)*
Crossing between potential energy surfaces in 2-(pyridin-2-yl) furan-3-ol

3PP-24 *Atsushi Horikoshi (Tokyo City University)*
On the external source method for Kubo-transformed quantum correlation functions

3PP-25 *Ikuo Fukuda (RIKEN)*
Zero-dipole summation method for precisely estimating electrostatic interaction in molecular dynamics

3PP-26 *Yusuke Ootani (RIKEN Advanced Institute for Computational Science)*
Ab initio molecular dynamics approach to tunneling splitting in polyatomic molecules

3PP-27 *Tomoko Akama (Waseda University)*
Short-time Fourier transform analysis of electron dynamics described by real-time TDHF

3PP-28 *Masato Sumita (National Institute for Materials Science)*
Computational study on photo- and thermo-reactions between tetra-tert-butyl-substituted cyclobutadiene and tetrahedrane

3PP-29 *Potjaman Poolmee (Kasetsart University)*
Photophysical properties and vibrational structure of ladder-type penta p-phenylene and carbazole derivatives based on SAC-CI calculations

3PP-30 *Shabbir Muhammad (Osaka University)*
Probing the multiradical character and nonlinear optical properties of linear and cyclic polyacenes: a wrapping effect in open-shell polyacenes

3PP-31 *Elizaveta Suturina (Institute of Chemical Kinetics and Combustion SB RAS)*
Reactivity of thiophenolate toward chalcogenadiazoles

3PP-32 *Yoshio Nishimoto (Nagoya University)*
Molecular and electronic structures of the super reduced state of a polyoxometalate (POM), $[Mo_{12}O_{40}P]^x$ (x = -3, -27)

3PP-33 *Marcus Lundberg (Uppsala University)*
Electronic structure of transition metal systems from X-ray spectroscopy

3PP-34 *Taku Onishi (Mie Univeristy)*
A theoretical study on proton conduction in nitrogen-doped $SrTiO_3$ perovskite

3PP-35 *Hirobumi Mineo (National Taiwan University)*
Application of the density matrix theory to the control of electronic ring current coupled to molecular vibrations in chiral molecule

3PP-36 *Mojmir Kyvala (Academy of Sciences of the Czech Republic)*
Inverse heavy-atom effect in conjugated carbenes, silylenes, aldehydes and ketones

3PP-37 *Hiroki Otaki (Kyoto University)*
Analysis of the effect of intermolecular interactions on dielectric properties in hydrogen-bonded material 5-bromo-9-hydroxyphenalenone

3PP-38 *Shigeyoshi Yamamoto (Chukyo University)*
Electronic states of GdF assigned in jj-coupling scheme

3PP-39 *Michiko Atsumi (Uppsala University)*
NMR shieldings of an excimer

3PP-40 *Kenji Sugisaki (Graduate School of Science, Osaka City University)*
Zero-field splitting tensors of nitroxide-based biradicals: A theoretical study

3PP-41 *Miho Otsuka (Ochanomizu University)*
Density functional theory calculations of iodine cluster anions: structures, chemical bonding nature, and vibrational spectra

3PP-42 *Takeshi Iwasa (JST-ERATO)*
A computational method for infrared reflection absorption spectroscopy

3PP-43 *Kota Daigoku (Kitasato University)*
Photoinduced charge-transfer and normal-cleavage reaction of Mg^+-benzene complex

3PP-44 *Michinori Sumimoto (Yamaguchi University)*
Theoretical study on the molecular structures of X-, α- and β-types of lithium phthalocyanine

3PP-45 *Soichi Shirai (Toyota Central R&D Laboratories, Inc.)*
Ab initio studies of aromatic excimers using multiconfiguration quasi-degenerate perturbation theory

3PP-46 *Toshihiko Abe (The University of Tokyo)*
Applying residual minimization method to GIAO-CPHF equation convergence for calculation of nuclear magnetic shielding tensors

3PP-47 *Hongyan Xiao (Kyoto University)*
A theoretical study on the photodissociation of HNO_3 involving S_2, S_1 and S_0 states

3PP-48 *Shinya Tsukamoto (Kyoto University)*
Theoretical study of luminescent vapochromic complexes including $AuCu_2(NHC)_2$ core

3PP-49 *Gergely Juhasz (Kyushu University)*
Intersystem crossing in spin-crossover complexes

3PP-50 *Koji Ohta (National Institute of Advanced Industrial Science and Technology (AIST))*
Theoretical study on two-photon absorption properties of two-dimensionally extended π-conjugated systems

3PP-51 *Hitomi Suto (Ochanomizu University)*
Structures and binding properties of noble gas compounds: NgBeO and $NgBeOBH_3$ (Ng = He, Ne, Ar)

3PP-52 *Masayuki Nakagaki (Kyoto University)*
Theoretical study of inverted sandwich type dinuclear complexes of ethylene and dinitrogen molecules

3PP-53 *Yoshihito Shiota (Kyushu University)*
Theoretical study of the mechanism of valence tautomerism in cobalt complexes

3PP-54 *Yuko Wasada-Tsutsui (Nagoya Institute of Technology)*
Density functional study of NO binding to Co-center in N_2S_2 coordination environment

3PP-55 *Nobuaki Tanaka (Shinshu University)*
DFT study of the properties and formation mechanism of 2-hydroxyterephthalate dianion

3PP-56 *Cristopher Camacho (Nagoya University)*
Theoretical interpretation of the photophysical properties of [n]cycloparaphenylenes

3PP-57 *Terutaka Yoshizawa (Kyoto University)*
NMR calculations of transition metal complexes containing M≡P triple bond

3PP-58 *Takashi Kawakami (Osaka University)*
Calculation of magnetic constants D in zero-field splitting by ab initio methods

3PP-59 *Yutaka Imamura (Waseda Univeristy)*
Multiple core ionizations and their relaxation process induced by X-ray free-electron laser

3PP-60 *Nozomi Takagi (Kyoto University)*
Characteristic fluxional behavior and bonding nature of hydrogen-bridged bis(silylene)

3PP-61 *Yasushi Honda (Quantum Chemistry Research Institute (QCRI))*
SAC-CI study on excitation spectra of doublet molecules

3PP-62 *Azusa Muraoka (Meiji University)*
The internal configuration inversion of ortho-phenylene derivative

3PP-63 *Nadtanet Nunthaboot (Mahasarakham University)*
Simultaneous analyses of photoinduced electron transfer in the wild- and mutant-types of the FMN binding protein from desulfovibrio vulgaris, Miyazaki F.

3PP-64 *Takahide Matsuoka (Keio University)*
Theoretical study on angular momentum polarization of photofragment of ICl

3PP-65 *Alexander V. Glushkov (Odessa University)*
Quantum modeling the cooperative laser electron-gamma-nuclear effects in spectra of molecular systems

3PP-66 *Alexander V. Glushkov (Odessa University)*
Raman scattering of the light on metastable levels of diatomics with an account for nuclear motion contribution

3PP-67 *Jingyi Yan (University of British Columbia)*
Electric field can induce heterogeneous ice nucleation

3PP-68 *Alain Allouche (CNRS & Université de Provence)*
First principles investigations on lithium – graphite interactions

3PP-69 *Thanyada Rungrotmongkol (Chulalongkorn University)*
Computational studies of viral influenza A neuraminidase subtype N_1

3PP-70 *Peter A. Limacher (ETH Zurich)*
Linearly conjugated chains exposed to an electric field: A closer look on the polarizabilities obtained with several quantum chemical methods

3PP-71 *Nikita I. Vakula (M.V. Lomonosov Moscow State University)*
Molecular modeling of silver adsorption on α-quartz surface

3PP-72 *Toru Saito (Osaka University)*
Theoretical study of [2+2] cycloaddition of cyclopentyne and ehtylene: Multireference and broken-symmetry approach

3PP-73 *Jagadeesh Suriyaprakash (Osaka University)*
Structural study of alpha-tetragonal boron by computational method

3PP-74 *Mikiya Fujii (The University of Tokyo)*
Packing effects in organic donor-acceptor molecular heterojunctions

3PP-75 *Yuh Hijikata (Kyoto University)*
Theoretical study of interaction between gas molecule and paddle-wheel unit of MOF

3PP-76 *Akira Imamura (Hiroshima Kokusai Gakuin University)*
Electronic structures and molecular structures of polyynes

3PP-77 *Kyohei Yoneda (Osaka University)*
Structural dependence of the open-shell characters and second hyperpolarizabilities in one-dimensional systems composed of trigonal graphene nanoflake units

3PP-78 *Go Tei (Osaka Prefecture University)*
An efficient light-harvesting system to excite optically-forbidden states of molecular

3PP-79 *Nanami Seki (Hokkaido University)*
Theoretical study on electronic structures of μ-oxo-bridged manganese complex

Sunday, September 4 (18:30 - 20:30)

4PP-01 *Rahul Maitra (Indian Association for the Cultivation of Science)*
Development and implementation of a manifestly spin-free state-specific multi-reference coupled cluster (SS-MRCC) theory using a multi-exponential type of cluster expansion

4PP-02 *Debalina Sinha (Indian Association for the Cultivation of Science)*
Formulation and implementation of a state-specific multi-reference coupled-cluster (SS-MRCC) theory using an internally contracted reference function.

4PP-03 *Boris N. Plakhutin (Russian Academy of Sciences)*
Active CI space for ionized systems as defined by Koopmans' theorem

4PP-04 *Fan Wang (Sichuan University)*
Open-shell coupled-cluster theory with spin-orbit coupling

4PP-05 *Wei Li (Nanjing University)*
Multilevel extension of the cluster-in-molecule method for the chemical reactions of large molecules

4PP-06 *Henryk A. Witek (National Chiao Tung University)*
Multireference perturbation theory can predict a false ground state

4PP-07 *Moto Tarumi (Waseda University)*
Antisymmetric product of strongly orthogonal geminals (APSG): Its acceleration and extension to open-shell systems

4PP-08 *Masayuki Ochi (The University of Tokyo)*
Efficient algorithm of the transcorrelated method for periodic systems - feasible wavefunction-based approach for solids -

4PP-09 *Hideaki Ishikawa (Home)*
Numerical analysis for eigenvalue problems in quantum mechanics and atomic structure calculations

4PP-10 *Robert Izsak (Bonn University)*
An overlap fitted RIJCOSX theory

4PP-11 *Hirofumi Sato (Kyoto University)*
Development and applications of theoretical methods for solvated molecular system

4PP-12 *Mitsuo Shoji (University of Tsukuba)*
A new procedure for the calculation of electron transfer coupling matrix element

4PP-13 *Ye Cao (National University of Singapore)*
Charge transfer complexes of dihalogen molecules: From weak intermolecular interaction to dative bonds

4PP-14 *Kanjarat Sukrat (Chulalongkorn University)*
Cracking reaction of C_2-C_4 alkanes sorbed in ZSM-5

4PP-15 *Tomoo Miyahara (Quantum Chemistry Research Institutte)*
Giant SAC-CI: Application to proteins

4PP-16 *Joonho Park (Korea Advanced Institute of Science and Technology)*
Screening of metals for CO_2 capture in MOF with open-metal site through the first-principle

4PP-17 *Yasutaka Kitagawa (Osaka University)*
Combination of spin-restricted and spin-projected calculations for a geometry optimization of large biradical systems

4PP-18 *Tatsuji Sano (The University of Electro-Communications)*
Norm-conserving stochastic Hartree-Fock calculation on electronic states in molecules

4PP-19 *Milind M. Deshmukh (Kyoto University)*
Dispersion energy of van der Waals complex: Approximate evaluation with pair-wise correlation effect

4PP-20 *Hiroaki Umeda (National Institute of Natural Sciences)*
OpenMP/MPI hybrid parallelization of GAMESS

4PP-21 *Fengyi Liu (Kyoto University)*
Theoretical study on the working mechanism of stilbene light-driven molecular rotary motor

4PP-22 *Michio Katouda (Institute for Molecular Science)*
Massively parallel second-order Møller–Plesset perturbation calculations based on divide-and-conquer method

4PP-23 *Takuma Yamamoto (Keio University)*
Calculation of rate constant for excitation energy transfer by Fermi's golden rule

4PP-24 *Takeshi Yoshikawa (Waseda University)*
Divide-and-conquer symmetry-adapted cluster method

4PP-25 *Lukman Hakim (Okayama University)*
Fast diffusion of water confined between plane surfaces coated with water monolayer

4PP-26 *Lukman Hakim (Okayama University)*
On the thermodynamic stability of hydrogen hydrates of ice Ic and ice II structures: A theoretical and simulation study

4PP-27 *Marzio Rosi (University of Perugia)*
Theoretical study of reactions relevant for atmospheric models of Titan: Excited nitrogen atoms with methane, ethene and ethane

4PP-28 *Masato Senami (Kyoto University)*
Description of time evolution and dielectric response based on rigged QED

4PP-29 *Oscar Olvera-Neria (Universidad Autonoma Metropolitana Azcapotzalco)*
A comparative ab initio multireference Møller-Plesset perturbation study for N_2O binding and activation by atomic excited states of Au, Pd, Pt and Rh

4PP-30 *Yoshiumi Kawamura (Toyota Motor Corporation)*
First principle calculation for hydriding reaction of metal boride

4PP-31 *Akinobu Shiga (Tokyo-Institute of Technology)*
Paired interacting orbitals (PIO) analysis of phenoxyimine-based olefin polymerization

4PP-32 *Takehiro Yoshikawa (Saitama University)*
Quantum tautomerization in porphycene and its istopomers: Path-integral molecular dynamics simulations

4PP-33 *Masaki Okoshi (Waseda University)*
Acceleration of CASSCF-MD simulation and its application to intramolecular charge transfer

4PP-34 *Hiroyuki Teramae (Josai University)*
Theoretical study on the reaction mechanism of formation of 3,5-diacetyl-1,4-dihydrolutidine

4PP-35 *Noriko Tsuchida (Ochanomizu University)*
DFT study of methyl/halogen exchange reaction on Pt complexes with phosphine ligand

4PP-36 *Takayuki Fujiwara (Rikkyo University)*
FMO-MD simulations for hydrated trivalent lanthanide ions using 4f-in-core model core

4PP-37 *Tomokazu Tanaka (Saitama University)*
Quantum dynamics study of the MuFF reaction system

4PP-38 *Shuichi Sugawara (Saitama University)*
Quantum proton transfer in hydrated sulfuric acid clusters

4PP-39 *Guixiang Zeng (Fukui Institute for Fundamental Chemistry, Kyoto University)*
Noble features in oxidative addition of B—Br σ—bond of bromoborane to $M(PMe_3)_2$ (M= Pt or Pd): Theoretical study

4PP-40 *Daisuke Yokogawa (Institute for Protein Research, Osaka University)*
Theoretical study on aquation reaction of cis-platin complex using RISM-SCF-SEDD

4PP-41 *Xue-fang Yu (Hokkaido University)*
Theoretical study of the mechanism of the excited-state double proton transfer in 7-azaindole dimer

4PP-42 *Shinji Aono (Fukui Institute for Fundamental Chemistry, Kyoto University)*
Solvation effect on hydrolysis of cis- and trans-platins

4PP-43 *Ken Sakata (Hoshi University)*
Ruthenium-catalyzed [3+2] cycloaddition via ruthenium-allenylidene intermediate: A DFT

4PP-44 *Masahiro Kunimoto (Waseda University)*
Theoretical study on catalytic activity of metal surfaces on P-H bond cleavage of

4PP-45 *Yasumitsu Suzuki (The University of Tokyo)*
Towards the development of the TD effective nuclear potential for time-dependent multicomponent density functional theory

4PP-46 *Junko Takahashi (University of Leiden)*
Molecular dynamics study of the photodesorption process of the CO molecule from the surface of interstellar ice

4PP-47 *Yu Harabuchi (Hokkaido University)*
Theoretical study of bifurcating reactions accompanying the totally-symmetric valley-ridge inflection point

4PP-48 *Jakob Petersen (Technical University of Denmark)*
Photodissociation, geminate recombination, and vibrational relaxation of iodine in carbon tetrachloride: A molecular dynamics simulation

4PP-49 *Karan Bobuatong (Institute for Molecular Science)*
Theoretical study on dehydrogenation reaction of methanol on anionic Au cluster

4PP-50 *Pornpan Pungpo (Ubon Ratchathani University)*
Molecular dynamics simulations of azanaphthoquinone annelated pyrrole derivatives as anti-cancer agent in DNA duplex

4PP-51 *Auradee Punkvang (Ubon Ratchathani University)*
Molecular modeling on anti-tuberculosis agent to investigate the structural basis for improving potency against M. tuberculosis strain

4PP-52 *My Hoa Nguyen (Vietnam National University, Hanoi (VNU))*
Study on the mechanism for the reaction of PBP2a with beta-taclam inhibitors by ONIOM

4PP-53 *ryo watanabe (Ibaraki University)*
Molecular dynamics study on complex between prostacyclin synthetase and prostaglandin H_2

4PP-54 *Kyohei Hanaoka (University of Tsukuba)*
Computational analysis for DNA religating reaction by E.coli topoisomerase IA

4PP-55 *Yu Takano (Osaka University)*
Density functional study of electronic structures of a characteristic [4Fe-4S] cluster, $[Fe_4S_4(SCH_3)_3(CH_3COO)]$, in dark-operative protochlorophyllide oxidoreductase

4PP-56 *Zhi-Qiang You (Academia Sinica)*
Ab inito study on triplet excitation energy transfer in photosynthetic light harvesting

4PP-57 *Yasuhiro Shigemitsu (Industrial Technology Center of Nagasaki)*
Quantum chemical study on molecular-level affinity of DJ-1 binding compounds

4PP-58 *Takao Otsuka (RIKEN)*
Theoretical study on hydrated DNA systems by linear-scaling DFT code CONQUEST

4PP-59 *Masaaki Saitow (Rikkyo University)*
Electronic excited state of a series of porphyrin molecules: Development of an effective renormalization scheme

4PP-60 *Yuka Koyama (Ochanomizu University)*
Interaction analysis of HIV-1 antibody 2G12 and glycans using FMO calculations

4PP-61 *Tomoyuki Iwase (University of Tsukuba)*
Fragment-DFT calculation on the interaction energy between HIV-1 protease and its inhibitor

4PP-62 *Lina Ding (Kyoto University)*
Theoretical study on the photo-decarboxylation mechanism of Green fluorescent protein

4PP-63 *Takefumi Yamashita (University of Tokyo)*
Effects of phospholipid bilayers on the hydrated excess proton behavior: A computational

4PP-64 *Osamu Miyashita (University of Arizona)*
Effect of crystal packing on protein conformation and dynamics

4PP-65 *Kaori Ueno-Noto (Kitasato University)*
A theoretical analysis on the interaction between Siglec-7 and its ligand by molecular dynamics and ab initio FMO method

4PP-66 *Tatsuya Joutsuka (Kyoto University)*
Electron transfer from cytochrome f to plastocyanin

4PP-67 *Toru Matsui (Osaka University)*
Structural properties and imino proton acidity of silver containing 5-substituted uracils

4PP-68 *Hirotaka Nishioka (Kyoto University)*
Electronic coupling calculation and pathway analysis of electron transfer reaction by using ab initio fragment-based method

4PP-69 *Patchreenart Saparpakorn (Waseda University)*
Application of DC-MP2 method to investigate the interaction energy of MK4965 in HIV-1 RT binding pockets

4PP-70 *Hiroaki Saito (Kanazawa University)*
Binding free energy of oxidized azurin–reduced cytochrome c551 complex

4PP-71 *Masanori Yamanaka (Nihon University)*
Towards making periodic table of motifs in irreducible decomposition of protein folding

4PP-72 *Ryo Akiyama (Kyushu University)*
Effect of multivalent ion on attractive interaction between like-charged macromolecules immersed in an electrolyte solution

4PP-73 *Kaori Fukuzawa (Mizuho Information & Research Institute Inc.)*
Fragment molecular orbital study for interaction between influenza virus neuraminidase and antiviral drug

4PP-74 *Jun Ohnuki (Waseda University)*
Energetical validation of the cleft open-close and the lever-arm swing of molecular motor

4PP-75 *Yuta Tsuji (Kyushu University)*
Orbital views of molecular conductance perturbed by anchor units

4PP-76 *Hiroyuki Tamura (Tohoku University)*
Quantum dynamics for organic solar cells

4PP-77 *Joonghan Kim (Fukui Institute for Fundamental Chemistry, Kyoto University)*
Determination of local chirality of irregular single-walled carbon nanotube based on individual hexagons

4PP-78 *Haibei Li (Kyoto University)*
Fullerene formation from hydrocarbon combustions: Quantum chemical molecular dynamics

4PP-79 *Tatsuhiko Ohto (The University of Tokyo)*
First-principles study of STM-induced melamine/Cu(001) switch: Energy barrier change with bias and various tip positions

4PP-80 *Eugene S. Kryachko (Bogolyubov Institute for Theoretical Physics)*
Functional features of voids of nanosized golden fullerenes

4PP-81 *Shotaro Watanabe (University of Tsukuba)*
Theoretical investigation of charge-transport properties in organic single crystals from constrained density functional theory

4PP-82 *Min Gao (Hokkaido University)*
Catalytic activity of gold clusters on the "inert" h-BN surface

4PP-83 *Ying Wang (Nagoya University)*
QM/MD simulations of graphene hydrogenation

4PP-84 *Noriyuki Mizoguchi (Meiji Pharmaceutical University)*
Finite length armchair carbon nanotubes: HOMO-LUMO gap oscillation and conjugated circuit

4PP-85 *Alexander V. Glushkov (Odessa University)*
Relativistic quantum chemistry of heavy elements, hadronic atoms and heavy ions collisions