Poster Session I (May 24)

PI-01 *Theoretical Study of Ion Pairing in Protic Ionic Liquids of ΔpKa = 6-18*

Allan L. L. East[1]

[1]Dept. of Chemistry and Biochemistry, University of Regina, Regina, Canada

PI-02 *Extending DFTB for Charge Transfer Studies under an Electric Field*

Ji Huang,[1] **Tim Kowalczyk**,[2] **Yoshio Nishimoto**,[3] **Daisuke Yokogawa**[1]

[1]Graduate School of Arts and Sciences, The University of Tokyo, Tokyo, Japan, [2]Department of Chemistry, Western Washington University, Bellingham, WA, United States, [3]Graduate School of Science, Kyoto University, Kyoto, Japan

PI-03 *Accurate calculation of hyper-Raman spectra in solution*

Kayo Suda,[1] **Kiyoshi Yagi**,[2] **Daisuke Yokogawa**[1]

[1]Graduate School of Arts and Sciences, The University of Tokyo, Tokyo, Japan, [2]Department of Chemistry, Institute of Pure and Applied Sciences, University of Tsukuba, Ibaraki, Japan

PI-04 *Analytical complex polarizability gradients for modeling resonance Raman spectroscopy*

Josefine H. Andersen,[1] **Iulia E. Brumboiu**,[2] **Patrick Norman**[1]

[1]Theoretical Chemistry and Biology, KTH Royal Institute of Technology, Stockholm, Sweden, [2]Institute of Physics, Nicolaus Copernicus University in Toruń, Toruń, Poland

PI-05 *Theoretical tautomer prediction as a testbed for theory-based experimental uncertainty analysis*

Michael Strobl,[1] **Nicolas Tielker**,[1] **Christian Chodun**,[1] **Stefan M. Kast**[1]

[1]Dept. of Chemistry and Chemical Biology, TU Dortmund University, Dortmund, Germany

PI-06 *Assessment of the time correlation function-based approach for absorption spectrum calculations using time-dependent density functional theory and molecular dynamics simulations*

Shion Sendo,[1] Kazuhiro J. Fujimoto,[1, 2] Tomoya Miyashita,[1] Shinji Saito,[3,4] Takeshi Yanai[1,2]

[1]Department of Chemistry, Graduate School of Science, Nagoya University, Aichi, Japan, [2]Institute of Transformative Bio-Molecules (WPI-ITbM), Nagoya University, Aichi, Japan, [3]Institute for Molecular Science, Aichi, Japan, [4]The Graduate University for Advanced Studies (SOKENDAI), Aichi, Japan

PI-07 *A semiclassical path Integral approach to vibrational spectra*

Motoyuki Shiga[1]

[1]Japan Atomic Energy Agency

PI-08 *Water Dynamics under Sub- and Supercritical Conditions*

Bo Thomsen,[1] Motoyuki Shiga[1]

[1]Center for Computational Science & e-Systems, Japan Atomic Energy Agency, Japan

PI-09 ~~*Quantum Monte Carlo study on positron binding to atomic anion dimers*~~

Moved to PIII-42

~~**S. Ito,[1] D. Yoshida,[1,2] Y. Kita,[1] T. Shimazaki,[1] M. Tachikawa[1]**~~

~~[1]Graduate School of NanoBioScience, Yokohama City University, Japan, [2]Nishina Center for Accelerator-Based Science, RIKEN, Japan~~

PI-10 *Unraveling Knots of Entangled Electrons in Strongly Correlated Quantum Materials*

Shaun Weatherly,[1] Troy Van Voorhis[1]

[1]Massachusetts Institute of Technology (MIT), Massachusetts, USA

PI-11 *New Frontiers of Bootstrap Embedding for Realistic Chemical Applications*

Minsik Cho,[1] Troy Van Voorhis[1]

[1]Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States of America

PI-12 *Extending Bootstrap Embedding to Excited States*

Alexandra Alexiu,[1] Beck Hanscam,[1] Troy Van Voorhis[1]

[1]Massachusetts Institute of Technology, Cambridge, Massachusetts, USA

PI-13 *Multiscale Bootstrap Embedding for Quantum Computing*

Leah P Weisburn,[1] Minsik Cho,[1] Moritz Bensberg,[2] Oinam Romesh Meitei,[1] Markus Reiher,[2] Troy Van Voorhis[1]

[1]Massachusetts Institute of Technology, [2]ETH Zurich

PI-14 *An Efficient, Black-Box Generation of Reaction Paths Via Redundant Internal Coordinates*

Noah C. Whelpley,[1] Troy A. Van Voorhis,[1] Oskar Weser[1]

[1]Massachusetts Institute of Technology, Boston, United States of America

PI-15 *Illustrating the usefulness of localized molecular orbitals in single and multi-reference embedding theories*

Souloke Sen,[1,2] Bruno Senjean,[3] Emiel Koridon,[1,2] Stefano Polla,[1] Lucas Visscher[2]

[1]Instituut-Lorentz, Universiteit Leiden, 2300RA Leiden, The Netherlands, [2]Theoretical Chemistry, Vrije Universiteit, 1081HV Amsterdam, The Netherlands, [3]ICGM,Université de Montpellier, CNRS, ENSCM, Montpellier, France

PI-16 *Electric Dipole Polarizability Calculation for Periodic and Non-periodic Systems using Atomic-Orbitals-based Linear Response Theory*

Ravi Kumar,[1,2] Sandra Luber,[1] Hirotaka Kitoh-Nishioka[2]

[1]Department of Chemistry, University of Zürich, Winterthurerstrasse 190, 8057 Zürich, Switzerland, [2]Department of Energy and Materials, Kindai University (Higashi Osaka Campus), Higashiosaka city, Osaka, Japan

PI-17 *Spintronic Properties of Antiferromagnetic and Ferromagnetic Triangulene-based Molecular Junctions*

Ameet Kumar,[1] Daeheum Cho[1]

[1]Department of Chemistry and Green-Nano Materials Research Center, Kyungpook National University, Daegu, South Korea

PI-18 *Photochemistry of Schiff Base Retinal and the Control of Dynamics using Optical Cavity*

Salman U Zaman,[1] Daeheum Cho[1]

[1]Department of Chemistry, Kyungpook National University, Daegu 41566, South Korea

PI-19 *Chiral-Induced Spin Selectivity in Photon-Coupled Achiral Matters*

Nguyen Thanh Phuc[1]

[1]Department of Molecular Engineering, Kyoto University, Kyoto, Japan

PI-20 *Generalized transition moment toward optimal excited states control with near-field*

Takeshi Iwasa[1]

[1]Department of Chemistry, Faculty of Science, Hokkaido University, Sapporo, Japan

PI-21 *Cavity-induced Modulation of Magnetic Properties: Insights into Molecular Aromaticity*

Alberto Barlini,[1] Andrea Bianchi,[1] Enrico Ronca,[2] Henrik Koch[3]

[1]Scuola Normale Superiore, Pisa 56126, Italy, [2]Dipartimento di Chimica, Biologia e Biotecnologie, Università degli Studi di Perugia, Perugia 06123, Italy, [3]Department of Chemistry, Norwegian University of Science and Technology, Trondheim 7491, Norway

PI-22 *PhasedInt: a Gaussian basis integral library with complex phase support*

Andrea Bianchi,[1] Enrico Ronca,[2] Henrik Koch[3]

[1]Scuola Normale Superiore, Pisa, Italy, [2]Università degli studi di Perugia, Perugia, Italy, [3]Norwegian University of Science and Technology, Trondheim, Norway

PI-23 *Excited-State Reaction Dynamics of Salicylideneaniline Molecules: Influence of the Molecular Crystalline Environment*

Hiroto Komuro,[1] Kenichiro Saita,[2] Takuro Tsutsumi,[2] Tetsuya Taketsugu[2,3]

[1]Graduate School of Chemical Sciences and Engineering, Hokkaido University, Japan, [2]Faculty of Science, Hokkaido University, Japan, [3]WPI-ICReDD, Hokkaido University, Japan

PI-24 *DC-MP2-PBC: Scalable ab initio calculation for large-scale periodic systems*

Gen Ogawa,[1] Masatsugu Nishida,[1] Tomoko Akama,[1] Masato Kobayashi,[1] Tetsuya Taketsugu[1]

[1]Hokkaido University, Japan

PI-25 *Matrix factorization analysis of OER in-situ Raman spectra and quantum chemical approach toward elucidating the activation mechanism of electrocatalysts*

Takeru Kojima,[1] Keisuke Tashiro,[2] Kenko Tsuchimoto,[1] Tomohiro Fukushima,[2] Kei Murakoshi,[2] Tetsuya Taketsugu,[2] Masato Kobayashi[2]

[1]Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo, Japan, [2]Faculty of Science, Hokkaido University, Sapporo, Japan

PI-26 *Divide and conquer projected UHF method for static electron correlation calculation of large systems.*

Sousei Kasaya,[1] Masatsugu Nishida,[1] Masato Kobayashi,[2,3] Tetsuya Taketsugu[2,3]

[1]Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo, Japan, [2]Faculty of Science, Hokkaido University, Sapporo, Japan, [3]WPI-ICReDD, Hokkaido University, Sapporo, Japan

PI-27 *Unraveling the excited-state dynamics of ortho-nitrophenol: insights from the surface hopping molecular dynamics and the reaction space projector (ReSPer) analysis*

Satoi Wada,[1] Takuro Tsutsumi,[1] Kenichiro Saita,[1] Tetsuya Taketsugu[1,2]

[1]Department of Chemistry, Faculty of Science, Hokkaido University, Japan, [2]WPI-ICReDD, Hokkaido University, Japan

PI-28 *Unraveling Dynamical Reaction Mechanisms in Bis-, Tris-, and Tetra-pericyclic Reactions: Reaction Space Projector Analysis*

Takuro Tsutsumi,[1] Keita Mataki,[2] Tatsuhiro Nakanishi,[2] Yuriko Ono,[3] Tetsuya Taketsugu[1,3]

[1]Department of Chemistry, Faculty of Science, Hokkaido University, Japan, [2]Graduate School of Chemical Sciences and Engineering, Hokkaido University, Japan, [3]WPI-ICReDD, Hokkaido University, Japan

PI-29 *Understanding Reaction Path Bifurcation Mechanisms Based on Electron Movement: Application of the Natural Reaction Orbital Method*

Tatsuhiro Nakanishi,[1] Takuro Tsutsumi,[2] Yuriko Ono,[3] Kazuki Sada,[2] Tetsuya Taketsugu[2,3]

[1]Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo, Japan, [2]Department of Chemistry, Faculty of Science, Hokkaido University, Sapporo, Japan, [3]WPI-ICReDD, Hokkaido University, Sapporo, Japan

PI-30 *Exploration of structural model of graphene oxide using GRRM*

Yasumasa Imai,[1] Takehiko Sasaki[1]

[1]Graduate School of Frontier Sciences, The University of Tokyo, Chiba, Japan

PI-31 *Advancing high-efficiency and stable blue OLEDs through computational materials design*

Kun-Han Lin,[1] Fang-Ting Liang,[1] Chong-Kai Niou,[1] Yao-Yu Lee[1]

[1]Department of Chemical Engineering, National Tsing Hua University, Hsinchu, Taiwan

PI-32 *First-Principles Study on Carrier Dynamics in Ge-Doped Sn Perovskites*

Koichi Yamashita[1]

[1]Yokohama City University, Japan

PI-33 *Unveiling the Reaction Mechanism of CO_2 Reduction on Bismuth-Based Perovskite $Cs_3Bi_2Br_9$: A Theoretical Study*

Pei Zhao,[1] Masahiro Ehara[1]

[1]Research Center for Computational Science, Institute for Molecular Science, Okazaki, Japan

PI-34 *Theoretical study on the four-electron oxidation mechanism of cobalt oxide catalysts*

Azusa Muraoka,[1] Narumi Fujiwara,[1] Koichi Yamashita[2]

[1]Graduate School of Science, Japan Women's University, Kyoto University, Tokyo, Japan, [2]Graduate School of Nanobioscience, Yokohama City University, Kanagawa, Japan

PI-35 *Molecular insight into C−C bond cleavage of alkanes on Ru surfaces based*

on free energy landscape

Kenshin Takei,[1] Tatsushi Ikeda,[1] Koki Muraoka,[1] Akira Nakayama[1]

[1]Department of Chemical System Engineering, The University of Tokyo, Tokyo 113-8656, Japan

PI-36 *Microscopic Structure and Proton Hopping Mechanisms at the Water/ZrO_2 Interface*

Tori Oishi,[1] Tatsushi Ikeda,[1] Akira Nakayama[1]

[1]Department of Chemical System Engineering, The University of Tokyo, Tokyo 113-8656, Japan

PI-37 *Discriminability and robustness of crystal structure identifiers using graphs*

Taku Tanimoto,[1] Koki Muraoka,[1] Tsubasa Munekata,[1] Akira Nakayama[1]

[1]Department of Chemical System Engineering, The University of Tokyo, Tokyo113-8656, Japan

PI-38 *Improving the accuracy-cost ratio in first-principles polymorph ranking for real-life molecular materials*

Ctirad Červinka,[1] Veronika Kostková,[1] Jan Ludík,[1] Petr Touš[1]

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PI-39 *Theoretical investigation of CO oxidation over polyoxometalate-supported Au cluster catalyst*

Tomohisa Yonemori,[1] Mitsutaka Okumura[1]

[1]Department of Chemistry, Osaka University, Osaka, Japan

PI-40 *A DFT study of the support dependence of propylene epoxidation over gold-supported catalysts*

Yasutaka Hamada,[1] Takashi Kawakami,[1] Shusuke Yamanaka,[1] Mitsutaka Okumura[1]

[1]Department of Chemistry, Graduate School of Science Osaka University, Osaka, Japan

PI-41 *Theoretical investigation of allyl alcohol isomerization over NiO and $LaNiO_3$-supported Au catalysts*

Yuhki Ishimaru,[1] Tamao Ishida,[2] Makoto Tokunaga,[3] Mitsutaka Okumura[1]

[1]Department of Chemistry, Osaka University, Osaka, Japan, [2]Department of Applied Chemistry for Environment, Tokyo Metropolitan University, Tokyo, Japan, [3]Department of Chemistry, Kyushu University, Fukuoka, Japan

PI-42 *Transition metal doped pyrazine-graphyne for high-performance CO2 reduction reaction to C1 products*

Rongwei Ma,[1,2] Yuejiao Yang,[1] Xinru Wei,[1] Daeheum Cho,[2] Jin Yong Lee,[3] Baotao Kang[1]

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PI-43 *Electronic Structure and Dynamics of Excitons in $CuFeO_2$*

Xuyan Ma,[1] Michel Dupuis[1]

[1]Department of Chemical and Biological Engineering, University at Buffalo, Buffalo, USA

PI-44 *Roles of Alkyl Group in Y6-base non fullerene acceptor and PM6 donor heterojunction*

Seungjun Jeong,[1] Daeheum Cho[1]

[1]Department of Chemistry and Green-Nano Materials Research Center, Kyungpook National University, Daegu, South Korea

Poster Session II (May 26)

PII-01 *Jahn–Teller Effect in Isomerization of Cubane*

Junki Sugimura,[1,2] Naoki Haruta,[1,2] Hiyori Takebe,[2,3] Seijiro Matsubara,[2,4] Tohru Sato[1,2]

[1]Fukui Institute for Fundamental Chemistry, Kyoto University, [2]Graduate School of Engineering, Kyoto University, [3]Academic Center for Computing and Media Studies, Kyoto University, [4]Institute of Liberal Arts and Sciences, Kyoto University

PII-02 *Effect of Mechanical Force on Yields and Selectivities of Diels–Alder Reactions*

Wakana Sakai,[1,2] Lori Gonnet,[3,4] Naoki Haruta,[1,2] Tohru Sato,[1,2] Michel Baron[3]

[1]Fukui Institute for Fundamental Chemistry, Kyoto University, [2]Graduate School of Engineering, Kyoto University, [3]Université de Toulouse, IMT Mines Albi, [4]School of Chemistry, University of Birmingham

PII-03 *Reassignment of the Vibronic Structure in the Absorption Spectrum of Carbon Cluster Anion C_6^- Exhibiting Fast Radiative Cooling*

Tetsuri Takami,[1,2] Naoki Haruta,[1,2] Tatsuhisa Kato,[1] Tohru Sato[1,2]

[1]Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto, Japan, [2]Graduate School of Engineering, Kyoto University, Kyoto, Japan

PII-04 *Theoretical Origin of Efficient Near-Infrared Emission of Triphenylamine-Benzothiadiazole Derivative*

Zhengnan Hu,[1,2] Naoki Haruta,[1,2] Tohru Sato[1,2]

[1]Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto, Japan, [2]Graduate School of Engineering, Kyoto University, Kyoto, Japan

PII-05 *Raman scattering theory based on the crude adiabatic representation*

Takumi Yagi,[1,2] Wataru Ota,[1,2] Naoki Haruta,[1,2] Tohru Sato[1,2]

[1]Graduate School of Engineering, Kyoto University, Kyoto, Japan, [2]Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto, Japan

PII-06 *Machine learning matrix product state wavefunction ansatz for strongly correlated systems*

Mandira Dey,[1] Debashree Ghosh[1]

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PII-07 *Deciphering the mechanism of singlet fission in carotenoids*

Supriyo Santra,[1] Debashree Ghosh[1]

[1]Indian Association for the Cultivation of Science, Jadavpur, Kolkata, India

PII-08 *Theoretical study on singlet fission dynamics in symmetric linear heterotrimer models consisting of 6,13-disubstituted pentacene derivatives*

Ryohei Kishi,[1,2,3] Hajime Miyamoto,[1] Kenji Okada,[1] Kohei Tada[1] Yasutaka Kitagawa[1,2,3,4]

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PII-09 *Magnetic coupling of one-dimensional radical chains in crystals investigated by approximate spin-projected density functional theory with plane-wave basis*

Kohei Tada,[1] Yukitika Kitano,[1] Ryohei Kishi,[1] Yasutaka Kitagawa[1]

[1]Graduate School of Engineering Science, The University of Osaka, Osaka, Japan

PII-10 *Theoretical study on relationship between structure and magnetic property of dysprosium(III) metallocene complex*

Yasutaka Kitagawa,[1,2,3,4,5] Koki Masuda,[1] Kaito Taka,[1] Ren Inoue,[1] Kohei Tada,[1] Ryohei Kishi[1,2,3,5]

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PII-11 *Control of the electronic state of surface-adsorbed double-decker yttrium(III)-phthalocyaninato complexes by changing the π-electron localization of ligands: A suggestion from DFT+U calculation*

Rikuya Hirota,[1] Kohei Tada,[1] Ryohei Kishi,[1] Yasutaka Kitagawa[1]

[1]Graduate School of Engineering Science, The University of Osaka, Osaka, Japan

PII-12 *Software development of essential ab initio simulator on quantum computers by first quantization*

Hideo Takahashi,[1] Tatsuya Tomaru,[2,3] Toshiyuki Hirano,[3,4] Saisei Tahara,[3] Fumitoshi Sato[3]

[1]School of Engineering, University of Tokyo, Japan, [2]Next Research, Research and Development Group, Hitachi Ltd., Japan, [3]Institute of Industrial Science, University of Tokyo, Japan, [4]Tokyo Metropolitan College of Industrial Technology, Japan

PII-13 *Accelerating Correlated Electronic Structure Calculations using Interpolative Separable Density Fitting*

Chia-Nan Yeh,[1] Miguel Morales[1]

[1]Center for Computational Quantum Physics, Flatiron Institute, Simons Foundation, New York, USA

PII-14 *Computing Excited States of Very Large Systems with Range-Separated Hybrid Functionals and the eXact Integral Simplified Time-Dependent Density Functional Theory (XsTD-DFT)*

Marc de Wergifosse[1]

[1]Theoretical Chemistry Group, Molecular Chemistry, Materials and Catalysis Division (MOST), Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, Place Louis Pasteur 1, B-1348 Louvain-la-Neuve, Belgium

PII-15 *Development of analytical energy gradient for Large-Scale Time-Dependent Density Functional Theory*

Muneaki Kamiya,[1,2] William Dawson,[2] Takahito Nakajima[2]

[1]Faculty of Regional Studies, Gifu University, 1-1 Yanagido, Gifu, Gifu 501-1193, Japan, [2]RIKEN Center for Computational Science, 7-1-26, Minatojima-minami-machi, Chuo-ku, Kobe, Hyogo 650-0047RIKEN, Japan

PII-16 *Can static correlation be described by single reference method?*

Stanislav Kedžuch,[1] Shota Tsuru,[1] Takahito Nakajima[1]

[1]RIKEN Center for Computational Science, Japan

PII-17 *Reducing Numerical Precision Requirements in Quantum Chemistry Calculations*

William Dawson,[1] Katsuhisa Ozaki,[2] Jens Domke,[1] Takahito Nakajima[1]

[1]RIKEN Center for Computational Science, [2]Shibaura Institute of Technology

PII-18 *Accuracy Meets Scalability for Computational Thermochemistry: The Family of Pisa Composite Schemes*

Silvia Di Grande,[1,2] Mihály Kállay,[3] Vincenzo Barone[4]

[1]Scuola Normale Superiore, Piazza dei Cavalieri 7, 56126 Pisa, Italy, [2]Scuola Superiore Meridionale, Largo San Marcellino 10, 80138 Napoli, Italy, [3]Budapest University of Technology and Economics, Műegyetem rkp. 3, 1111 Budapest, Hungary, [4]INSTM, via Giuseppe Giusti 9, 50121 Firenze, Italy

PII-19 *Accelerating Nanoparticle Catalyst Design Using Quantum-Inspired Algorithms*

Tuan Minh Do,[1] Tomoya Shiota,[1,2] Wataru Mizukami[1,2]

[1]Center for Quantum Information and Quantum Biology, The University of Osaka, Osaka, Japan, [2]Graduate School of Engineering Science, The University of Osaka, Osaka, Japan

PII-20 *Enhancing Quantum Power Methods with Generalized Quantum Signal Processing*

Viktor Khinevich,[1,2] Wataru Mizukami[1,2]

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PII-21 *Auxiliary-field quantum Monte Carlo method using a resource-efficient quantum-classical hybrid approach*

Yuichiro Yoshida,[1] Luca Erhart,[1] Takuma Murokoshi,[1] Rika Nakagawa,[2] Chihiro Mori,[2] Wataru Mizukami[1]

[1]Center for Quantum Information and Quantum Biology, Osaka University, Osaka, Japan, [2]Technology Strategy Center, TOPPAN Digital Inc., Tokyo, Japan

PII-22 *ADAPT-QSCI: Adaptive Construction of an Input State for Quantum-Selected Configuration Interaction*

Yuya O. Nakagawa,[1] Masahiko Kamoshita,[1] Wataru Mizukami,[2,3] Shotaro Sudo,[4] Yu-ya Ohnishi[4]

[1]QunaSys Inc., [2]Center for Quantum Information and Quantum Biology, Osaka University, [3]Graduate School of Engineering Science, Osaka University, [4]JSR Corporation

PII-23 *An Energy Decomposition Analysis of Intermolecular Interaction Energies from MP2 Theory*

Zhenling Wang,[1,2] Hengyuan Shen,[1,2] Martin Head-Gordon[1,2]

[1]Department of Chemistry, University of California, Berkeley, California, USA, [2]Chemical Sciences Division, Lawrence Berkeley National Lab, Berkeley, California, USA

PII-24 *Antisymmetry rules of response properties in certain chemical spaces*

Takafumi Shiraogawa,[1,2,3] Simon León Krug,[4] Masahiro Ehara,[1,2,3] O. Anatole von Lilienfeld[4,5,6,7,8,9,10]

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PII-25 *A useful basis for understanding chemistry*

Hengyuan Shen[1]

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PII-26 *Solvatochromism observed in the X-ray absorption spectrum of indole dissolved in water*

Shota Tsuru,[1] Masanari Nagasaka[2]

[1]RIKEN Center for Computational Science, RIKEN, Kobe, Japan, [2]Institute for Molecular Science, Okazaki, Japan

PII-27 *Solvent Effect on Z-(Allyloxycarbonyl)methyl Radical Cyclization: Influence of Solvation Structure*

Sara Suzuki,[1] Soni Aman Govind,[2] Kosuke Imamura,[1] Hideki Yorimitsu,[3] Hiroshi Shinokubo,[4] Masahiro Higashi,[5] Hirofumi Sato[1,6]

[1]Graduate School of Engineering, Kyoto University, Kyoto, Japan, [2]Indian Institute of Technology (BHU), [3]Graduate School of Science, Kyoto University, Kyoto, Japan, [4]Graduate School of Engineering, Nagoya University, Aichi, Japan, [5]Graduate School of Informatics, Nagoya University, Aichi, Japan, [6]Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto, Japan

PII-28 *Theoretical Study on Excitation Energy Transfer of Light-Harvesting Antenna using Exciton Model with Charge Transfer States and Their Fluctuations*

Shunsuke Yabu,[1] Hirofumi Sato,[1,2] Masahiro Higashi[3]

[1]Graduate School of Engineering, Kyoto University, Kyoto, Japan, [2]Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto, Japan, [3]Graduate School of Informatics, Nagoya University, Nagoya, Japan

PII-29 *First-Principles Investigation of Enhanced Water Splitting in Sr-Doped $NaTaO_3$*

Ryusei Morimoto,[1] Hiroki Uratani,[1,2] Hirofumi Sato[1,3]

[1]Graduate School of Engineering, Kyoto University, Japan, [2]PRESTO, Japan Science and Technology Agency (JST), Japan, [3]Fukui Institute for Fundamental Chemistry, Kyoto University, Japan

PII-30 *Construction of quasi-diabatic orbitals via time-dependent Kohn–Sham equations and its application to excited-state dynamics*

Hiroki Uratani,[1,2] Hirofumi Sato[1,3]

[1]Graduate School of Engineering, Kyoto University, Kyoto, Japan, [2]PRESTO, Japan Science and Technology Agency, Kawaguchi, Japan, [3]Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto, Japan

PII-31 *The stereoeletronic effects on the conformations of α-fluorinated dipeptide*

Hikaru Oshimo,[1] Kanami Sugiyama,[1] Genta Koja,[2] Tomohiro Agou,[3] Hisanori Arakaki,[4] Riko Genka,[4] Satoru Arimitsu,[5] Hirofumi Sato,[1,6] Masahiro Higashi[7]

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PII-32 *Theoretical investigation of NH_3 decomposition mechanism on GaN surface*

Kazuki Tsunoda,[1] Kanami Sugiyama,[1] Hirofumi Sato[1,2]

[1]Graduate School of Engineering, Kyoto University, Kyoto, Japan, [2]Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto, Japan

PII-33 *Systematic reaction path search and its analysis for trimethyl gallium decomposition with NH_3 and H_2*

Kanami Sugiyama,[1] Akira Kusaba,[2] Hirofumi Sato[1,3]

[1]Department of Molecular Engineering, Kyoto University, Kyoto, Japan, [2]Research Institute for Applied Mechanics, Kyushu University, Fukuoka, Japan, [3]Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto, Japan

PII-34 *Solvent effect on the UV circular dichroism of a tetrapeptide in aqueous solution using time-dependent density functional theory combined with reference interaction site model*

Yuji Takabayashi,[1] Hirofumi Sato[1,2]

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PII-35 *A Model Electronic Hamiltonian to Study Electronic States and Electronic Absorption Spectra of $[Ni(phen)_3]^{2+}$*

Leo Sugimula,[1] Satoru Iuchi,[2] Hirofumi Sato[1,3]

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PII-36 *Nucleobases in Water Clusters: From Initial Conditions to Photophysical Observables*

Antonio Prlj[1]

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PII-37 *Theoretical Insight into Catalytic Mechanism of GH11 Xylanase: ab initio QM/MM Modeling based on Neutron Structure*

Toyokazu Ishida,[1] Jerry M Parks,[2] Jeremy C Smith[2]

[1]National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan, [2]Center for Molecular Biophysics, Oak Ridge National Laboratory, Tennessee, United States

PII-38 *Dimensionality-Induced Effects on Transport Properties of Triangulene-Based Polymers and Molecular Junctions*

Hyungu Kang,[1] Iuliia Olshevskaia,[1] Daeheum Cho[1]

[1]Department of Chemistry and Green-Nano Materials Research Center, Kyungpook National University, Daegu 41566, South Korea

PII-39 *Exploration of the Origins of σ Interference*

Yuta Tsuji,[1] Kazuki Okazawa,[2] Toshinobu Tatsumi,[1] Kazunari Yoshizawa[3]

[1]Faculty of Engineering Sciences, Kyushu University, Kasuga, Japan, [2]Center for Computational Sciences, University of Tsukuba, Japan, [3]Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto, Japan

PII-40 *Coupled Cluster calculations of energies, structure and properties for larger symmetric molecules*

Luca Melega,[1] Tommaso Nottoli,[1] Jürgen Gauss,[2] Filippo Lipparini[1]

[1]Dipartimento di Chimica e Chimica Industriale, Università di Pisa, Italy, [2]Department Chemie, Johannes Gutenberg-Universität Mainz, Germany

PII-41 *A Concordant Mode Approach to Intermolecular Vibrations*

Laura N. Olive Dornshuld,[1] Mitchell E. Lahm,[1] Nathaniel L. Kitzmiller,[1] Wesley D. Allen,[1] Henry F. Schaefer III[1]

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PII-42 *Einsums: Simple High-Performance Tensor Contractions*

Connor Briggs,[1] Justin T. Turney,[1] Henry F. Schaefer, III[1]

[1]University of Georgia, Athens, Georgia, United States

PII-43 *Binding energy from umbrella sampling at ML-enhanced Born-Oppenheimer MD simulations*

Jakub Kubecka,[1] Georg Baadsgaard Trolle,[1] Yosef Knattrup,[1] Jonas Elm,[1] Ivo Neefjes[1]

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PII-44 *Bridging Ab-Initio Molecular Dynamics and Sustainable Biomass Transformation*

Radu Alexandru Talmazan,[1] Christophe Chipot,[1] Benoit Roux[2]

[1]Universite de Lorraine, [2]University of Chicago

Poster Session III (May 27)

PIII-01 *On the applicability of CCSD(T) for dispersion interactions in large conjugated systems*

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PIII-02 *Enabling OF-DFT with Machine Learning*

T. Kaczun,[1] R. Remme,[1] T. Ebert,[1] C. A. Gehrig,[1] D. Geng,[1] G. Gerhartz,[1] M. K. Ickler,[1] M. V. Klockow,[1] P. Lippmann,[1] J. S. Schmidt,[1] S. Wagner,[1] F. A. Hamprecht,[1] A. Dreuw[1]

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PIII-03 *Q-ADC(2): The Second-Order Algebraic Diagrammatic Construction Scheme for Electronic Excitations by Quadrature*

Antonia Papapostolou,[1] Andreas Dreuw[1]

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PIII-04 *Modeling electronic processes in open-shell molecules using ADC*

Adrian L. Dempwolff,[1] Marcus Alexandru,[1] Andreas Dreuw[1]

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PIII-05 *A Memory-Efficient Reformulation of ADC(4)*

Adrian Müller,[1] Dirk R. Rehn,[1] Andreas Dreuw[1]

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PIII-06 *Molecular Properties Employing ADC(2/1+)*

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PIII-07 *Analytic Derivatives of CASPT2/PCM in OpenMolcas*

Yoshio Nishimoto[1]

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PIII-08 *Driven similarity renormalization group with a large active space*

Chenyang Li,[1] Xiaoxue Wang,[1] Huanchen Zhai,[1] Wei-Hai Fang[1]

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PIII-09 *Multireference study of C-H activation - amination reaction mechanism on a di-Ru complex catalyst*

Maria Kosaka,[1] Yuki Kurashige[1,2,3]

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PIII-10 *Electron Spin-Lattice Relaxation and Dephasing Dynamics of Triplet Chromophores in a Host Crystal*

Katsuki Miyokawa,[1] Yuki Kurashige[1,2,3]

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PIII-11 *Multireference study of the optical spin polarization mechanism in organic and inorganic molecules*

Yuki Yamamoto,[1] Yuki Kurashige[2,3,4]

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PIII-12 *On-the-fly propagation of multi-configurational wave packets using the semi-classical propagator*

Masaya Tsumura,[1] Yuki Kurashige[1,2,3]

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PIII-13 *Explaining the Role of Spin-Orbit Coupling in Electron Spin Polarization Reversal of Metal-Complex Connected Systems*

Ryosuke Sowa,[1] Yuki Kurashige[1,2,3]

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PIII-14 *Calculation of vibrational state of water cluster on Pt surface taking account of anharmonicity*

Akari Takahashi,[1] Yuki Kurashige[1,2,3]

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PIII-15 *Quantum Chemical Density Matrix Renormalization Group Method Boosted by Machine Learning*

Pavlo Golub,[1] Chao Yang,[2] Vojtěch Vlček,[3] Libor Veis[1]

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PIII-16 *Density Matrix Renormalization Group Approach Based on the Coupled-Cluster Downfolded Hamiltonians*

Nicholas Bauman,[1] Libor Veis,[2] Karol Kowalski,[1] Jiri Brabec[2]

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PIII-17 *Projection-based DMRG-in-DFT embedding: non-additive exchange-correlation corrections by adiabatic connection*

Enzo Monino,[1] Daria Drwal,[2] Katarzyna Pernal,[2] Libor Veis[1]

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PIII-18 *Two Frontiers of Condensed Phase Quantum Chemistry: Ab Initio Polarons and Chemical Intuition*

Paul J. Robinson,[1] **Joonho Lee**[1]

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PIII-19 *Second-order Møller–Plesset perturbation theory with pair natural orbitals for periodic systems*

Andrew Zhu,[1] **Poramas Komonvasee**,[1] **Arman Nejad**,[1] **David Tew**[1]

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PIII-20 *The Relativistic Pseudopotential Correlation-Consistent Composite Approach (rp-ccCA) for Bond Dissociation Energies of 5d Transition Metal Diatomics*

Jaxon S. George,[1] **Bradley K. Welch**,[1] **Angela K. Wilson**[1]

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PIII-21 *Multicenter molecular integrals over Dirac wave functions for several fundamental properties*

Kazuhiro Ishida[1]

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PIII-22 *Scalable Parallel Algorithms of Two-Electron Integrals in Two-Component Relativistic Theory*

Chinami Takashima,[1] **Hiromi Nakai**[1,2]

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PIII-23 *Development of direct minimization method for SCF solution combining Givens rotation and error back propagation*

Rei Oshima,[1] **Hiromi Nakai**[1,2]

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PIII-24 *Geometry Optimization of Non-Local Excited States Using Divide-and-Conquer Method*

Ryusei Nishimura,[1] Takeshi Yoshikawa,[2,3] Ken Sakata,[2] Hiromi Nakai[1,3]

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PIII-25 *Analysis of supported metal nanoparticles using first principles calculation*

Miyu Onishi,[1] Ayako Nakata,[2] Hiromi Nakai[1,3]

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PIII-26 *Development of an approximate calculation method for highly excited states in lanthanide systems*

Soshi Ikuta,[1] Taichi Inagaki,[1] Miho Hatanaka[1,2]

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PIII-27 *Theoretical analysis of intermolecular vibrational motions of water at the water-air interface using molecular simulations*

Masaki Kondo,[1] Taichi Inagaki,[1] Miho Hatanaka[1,2]

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PIII-28 *Molecular insights into the hydration reaction of magnesium oxide*

Taichi Inagaki,[1] Miho Hatanaka[1,2]

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PIII-29 *Characterization of Enol Ether Intermediates in the Intramolecular Stetter Reactions by DFT and Kinetic Simulations*

Gou-Tao Huang,[1] Jen-Shiang K. Yu,[1,2,3]

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PIII-30 *Exploring Novel Oxidation Pathways of Volatile Organic Compounds Initiated by Acyl Peroxy Radicals*

Dominika Pasik,[1,2] Siddharth Iyer,[3] Nanna Myllys[1,2]

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PIII-31 *Molecular Mechanism of the formation of a semiquinone radical in Bacterial Copper Amine Oxidase*

Mitsuo Shoji,[1] Takeshi Murakawa,[2] Yasuteru Shigeta,[1] Hideyuki Hayashi,[2] Toshihide Okajima[3]

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PIII-32 *Exploring the Photolysis Mechanism of Propylene Oxide in Space using DFT/TD-DFT*

Manussada Ratanasak,[1] Yuta Hori,[1] Mitsuo Shoji,[1] Yasuteru Shigeta[1]

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PIII-33 *A Theoretical Study on the Rh-Catalyzed 2,3-Disubstituted Benzofuran Synthesis*

Hirona Itakura,[1,2] Ray Miyazaki,[2] Shohei Ono,[3,4] Keita Uehara,[3] Makoto Sako,[3] Mitsuhiro Arisawa,[3] Jun-ya Hasegawa[2]

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PIII-34 *Electronic structures and relative stability in the S_3 state of the $CaMn_4O_5$ cluster of the OEC by DFT and CC calculations*

Koichi Miyagawa,[1] Mitsuo Shoji,[1] Takashi Kawakami,[1] Kizashi Yamaguchi[1]

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PIII-35 *UNO (ULO) Classical and Quantum Computations of Mn Oxides Clusters*

Takashi Kawakami,[1] Koichi Miyagawa,[2] Mitsuo Shoji,[2] Hiroshi Isobe,[3] Kizashi Yamaguchi[4,5]

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PIII-36 *Hydration of atmospheric molecular clusters*

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PIII-37 *Zero-energy resonance in hydrogen dynamics and its impact on hydrogen debonding in materials*

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PIII-38 *Development of Relativistic CASPT2/RASPT2 Program along with DIRAC Software and Its application to UO_2^{2+}*

Yasuto Masuda,[1] Minori Abe[1]

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PIII-39 *Polaritonic Chemistry Using the Density Matrix Renormalization Group Method*

Mikulas Matousek,[1,2] Nam Vu,[3] Niranjan Govind,[4] Jonathan Jay Foley IV,[3] Libor Veis[1]

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PIII-40 *A unified framework for the automated derivation of quantum many-body theories*

Huanchen Zhai,[1] Garnet K. L. Chan[2]

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PIII-41 *Embedded multi-configurational electronic structure methods*

Fangcheng Wu,[1] Daniel Kats[1]

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PIII-42 *Quantum Monte Carlo study on positron binding to atomic anion dimers*

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