POSTERS

POSTER SESSION 1 – SUNDAY SEPTEMBER 14 – 4.30-6.30pm

PP001 **Adsorption and Photodegradation of Toluene by Application of Ultraviolet Irradiation on a New Adsorbent made by Microbial Cellulose using TiO_2 Nanoparticles**
Gholamhossein Pourtaghi[1], Abbas Rezaee[2], Ali Khavanin[2], Fariba Mohammadi[1], *[1]Baqayatallah University of Medical Sciences, Iran, Islamic Republic of, [2]Trabiat Modares University, Iran, Islamic Republic of*

PP002 **Sequence-Dependent Stability of DNA and Netropsin-DNA Complexes: Insights from Free Energy Calculations**
Jožica Dolenc[1], Chris Oostenbrink[2], Wilfred F. van Gunsteren[3], *[1]University of Ljubljana, Faculty of Chemistry and Chemical Technology, Slovenia; [2]Vrije Universiteit Amsterdam, Department of Pharmacochemistry, Netherlands*; *[3]Swiss Federal Institute of Technology, Laboratory of Physical Chemistry, Switzerland*

PP003 **Reactivity Comparison of Artemisinin and its Synthetic Derivatives: A DFT Approach**
Kalyan Kr. Hazarika[1], Nabin Ch. Barua[3], Ramesh Ch. Deka[2], *[1]Department of Molecular Biology & Biotechnology, Tezpur University, India, [2]Department of Chemical Sciences, Tezpur University, India, [3]Natural Products Chemistry Division, North East Institute of Science & Technology (CSIR), India*

PP004 **The Fragment Molecular Based Time-Dependent Density Functional Theory for Excitations in Large Systems**
Mahito Chiba[1], Dmitri Fedorov[1], Kazuo Kitaura[2], *[1]Research Institute for Computational Sciences, National Institute of Advanced Industrial Science and Technology (AIST), Japan, [2]Graduate School of Pharmaceutical Sciences, Kyoto University, Japan*

PP005 **Hydrogen Bonded Rings as Supramolecular Motifs**
Catharine Esterhuysen[1], Martin W. Bredenkamp[1], Leonard J. Barbour[1], *[1]University of Stellenbosch, Department of Chemistry and Polymer Science, South Africa*

PP006 **Amino Acid Residues and their Roles in the Chemistry of Protein Catalysis**
Gemma Holliday[1], Daniel Almonacid[2], John Mitchell[2], Janet Thornton[1], *[1]EMBL-EBI, United Kingdom, [2]Unilever Centre for Molecular Science Informatics, University of Cambridge, United Kingdom*

PP007 **A New Approach for Theoretical Analysis of Intramolecular Interactions**
Kenta Yamada[1], Nobuaki Koga[1], *[1]Nagoya University, Japan*

PP008 **Formation of a Hydrogen Bond with the Head Group is Important for Insecticidal and Neuroblocking Potencies of Imidacloprid-Related Neonicotinoids**
Yuji Naruse[1], Shinzo Kagabu[2], Keiichiro Nishimura[3], Ikuya Ohno[2], *[1]Department of Chemistry, Faculty of Engineering, Gifu University, Japan, [2]Department of Chemistry, Faculty of Education, Gifu University, Japan, [3]Institute for Advanced Science and Technology, Osaka Prefecture University, Japan*

PP009 **Application of the PFV EoS Correlation to Excess Molar Volumes of (1-Ethyl-3-methylimidazolium Ethyl Sulfate + Alkanols) at Different Temperatures and VLE Prediction**
Nirmala Deenadayalu[1], Sabyasachi Sen[2], *[1]Durban University of Technology, South Africa, [2]Invensys SimSci Esscor, United States*

PP010 **Multifarious-Magnetism in Copper Oxide Nanostructures from First-Principles**
Aloysius Soon[1], Xiang-Yuan Cui[1], Bernard Delley[2], Catherine Stampfl[1], *[1]School of Physics, The University of Sydney, Australia, [2]Paul-Scherrer-Institut, Switzerland*

PP011 **The Investigation of Two-Dimensional Semiconducting Nanostructures Based on Single Graphene Sheets with "Lines" of Adsorbed Hydrogen Atoms by the DFT Method**
Pavel Sorokin[1], Leonid Chernozatonskii[2], *[1]Siberian Federal University, Russian Federation, [2]Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, Russian Federation*

PP012 **BEBOP, A New Reactive Potential using Bond-Energy/Bond-Order Relationships**
Sonia Tulyani[1], Phillip R. Westmoreland[1], George A. Petersson[2], *[1]University of Massachusetts Amherst, United States, [2]Wesleyan University, Chemistry, United States*

PP013 **Modelling the Size, Shape and Self-Assembly CdSe Nanorods into High Aspect Quantum Wires**
Amanda Barnard[1], Huifang Xu[2], *[1]The University of Melbourne, School of Chemistry, Australia, [2]The University of Wisconsin-Madison, Department of Geology and Geophysics, United States*

Poster Session 1 – Sunday September 14 – 4.30-6.30pm

PP014 **The Rh-S Coordination Modes in Cyclometalated Dirhodium(II,II) Thienyl Phosphine Complexes**
Pipsa Hirva[1], Julio Lloret[2], Pascual Lahuerta[2], *[1]University of Joensuu, Department of Chemistry, Finland, [2]Universidad de Valencia, Departamento de Química Inorgánica, Spain*

PP015 **An ISC/IVR Study of the First Triplet State of Thiophosgene, Cl_2CS**
David Moule[1,2], *[1]Brock University, Department of Chemistry, Canada, [2]Institute of Solid State Physics, Bulgarian Academy of Sciences, Bulgaria*

PP016 **Molecular Dynamics Study of Amyloid Formation of Abl-SH3 Domain Peptides**
Inta Liepina[1], Salvador Ventura[2], Cezary Czaplewski[3], Adam Liwo[3], *[1]Latvian Institute of Organic Synthesis, Latvia, [2]Institut de Biotecnologia i de Biomedicina, Universitat Autonoma de Barcelona, Spain, [3]Faculty of Chemistry, University of Gdansk, Poland*

PP017 **1.4-DHP-Lipid Forms a Tubular Micellae**
Inta Liepina[1], Cezary Czaplewski[2], Velta Ose[3], Gunars Duburs[4], *[1]Latvian Institute of Organic Synthesis, Riga, Latvia and Center of Drug Research, University of Helsinki, Finland, [2]Faculty of Chemistry, University of Gdansk, Poland, [3]Latvian Biomedical Research and Study Centre, Latvia, [4]Latvian Institute of Organic Synthesis , Latvia*

PP018 **Hydration Structure and Dynamics of Lanthanides by Molecular Dynamics Simulations with a Polarizable Force Field**
Magali Duvail[1], Pierre Vitorge[2], Riccardo Spezia[1], *[1]Université d'Evry val d'Essonne, UMR CNRS 8586 LAMBE, France, [2]CEA Saclay, DEN/DPC/SECR/LSRM, France*

PP019 **Car-Parrinello Molecular Dynamics of Co(III) Cysteinato Complexes in Solution**
Riccardo Spezia[1], Marie-Pierre Gaigeot[1], *[1]Université d'Evry val d'Essonne, UMR CNRS 8586 LAMBE, France*

PP020 **Hyperbranched Polymer Melts: A Non-Equilibrium Molecular Dynamics Study**
Tu Le[1], Billy Todd[1], Peter Daivis[2], Alfred Uhlherr[3], *[1]Centre for Molecular Simulation, Swinburne University of Technology, Australia, [2]School of Applied Sciences, RMIT University, Australia, [3]Molecular Science, CSIRO, Australia*

PP021 **Investigation of HEME, HEME-O_2, the Transition State between them and their Dependence on a Dielectric Medium: IR Spectra and Thermodynamic Properties**
Mojgan Heshmat[1], *[1]Islamshahr Branch Islamic Azad University, Iran, Islamic Republic of*

PP022 **Aluminum Siting in Silicon-Rich Zeolite Frameworks: A Combined Experimental (High Resolution ^{27}Al NMR Spectroscopy) and Theoretical (DFT/MM) Approach**
Stepan Sklenak[1], *[1]J. Heyrovsky Institute of Physical Chemistry of ASCR, v.v.i., Czech Republic*

PP023 **Computational Study of Acylphloroglucinols – A Promising Class of Biologically Active Compounds**
Liliana Mammino[1], Mwadham Kabanda[1], *[1]University of Venda, Department of Chemistry, South Africa*

PP024 **Structural Stabilization and Onset of Acid Dissociation in Hydrogen Halide-Water Aggregates**
Marco Masia[1], Dominik Marx[2], *[1]Università di Sassari, Dipartimento di Chimica, Italy, [2]Ruh Universitaet Bochum, Lehrsthul für Theoretische Chemie, Germany*

PP025 **Theoretical Insights Into the Mechanism of Asymmetric Aldol Organocatalysis in Water**
Marco Masia[1], Jordi Ribas Ariño[2], Maria Àngels Carvajal Barba[3], *[1]Università di Sassari, Dipartimento di Chimica, Italy, [2]Ruh Universitaet Bochum, Lehrsthul für Theoretische Chemie, Germany, [3]The Hebrew University of Jerusalem, Organic Chemistry Department and Lise Meitner Center for Computational Chemsitry, Israel*

PP026 **Ab Initio Modelling of Cluster Distributions Generated by Mass Spectral Techniques**
Jason Sky[1], Ellak von Nagy-Felsobuki[1], *[1]The University of Newcastle, School of Environmental and Life Sciences, Australia*

PP027 **Ab Initio Rovibrational Spectra of Ion-Quadrupole Complexes**
Alister Page[1], Ellak von Nagy-Felsobuki[1], *[1]The University of Newcastle, School of Environmental and Life Sciences, Australia*

PP028 **Indenyl Ferrocenes – a Test of DFT Theory**
Robert Maclagan[1], Owen Curnow[1], *[1]Department of Chemistry, University of Canterbury, New Zealand*

PP029 **Melting of Nano Clusters using Adaptive Exchange Monte Carlo Simulations**
Elke Pahl[1], Florent Calvo[2], Peter Schwerdtfeger[1], [1]*Centre of Theoretical Chemistry and Physics (CTCP); The New Zealand Institute for Advanced Study, Bld.44, Massey University Auckland, New Zealand,* [2]*LASIM, Universite Claude Bernard Lyon 1, France*

PP030 **Electronic Structure, Metal-Metal Interactions, and Magnetic Properties of Mo and W ($[M_3X_{12}]^{3-}$) Halide Clusters**
Germán E Cavigliasso[1], Robert Stranger[1], [1]*Department of Chemistry, Faculty of Science, Australian National University, Australia*

PP031 **Exploring the Active Sites of Sirtuins, Anti-Ageing" Enzymes, by Docking Studies**
Maija Lahtela-Kakkonen[1], Heikki Salo[1], Tero Huhtiniemi[1], Päivi Kiviranta[1], Jukka Leppänen[1], Elina Jarho[1], Antero Salminen[2], Antti Poso[1], [1]*University of Kuopio, Department of Pharmaceutical chemistry, Finland,* [2]*University of Kuopio, Department of Neurology, Finland*

PP032 **Al- and Si-substituted Magnesium Hydrides as Hydrogen Storage Materials: A DFT Study**
Tuhina Kelkar[1], Sourav Pal[1], D. G. Kanhere[2], [1]*Physical Chemistry Division, National Chemical Laboratory, India,* [2]*Department of Physics and Center for Modeling and Simulations, University of Pune, India*

PP033 **Exploring the Mechanisms of Boiling and Distillation Processes**
Dirk Zahn[1], [1]*MPI CPfS, Germany*

PP034 **Active-Space Equation-of-Motion Coupled-Cluster Methods for Ground and Excited States of Radicals and Other Open-Shell Systems**
Jeffrey Gour[1], Piotr Piecuch[1], Masahiro Ehara[2], [1]*Department of Chemistry, Michigan State University, United States,* [2]*Department of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University, Japan*

PP035 **Ab Initio Relativistic Calculations of Isotope Fractionation in the U(III)–U(IV) Exchange Reaction**
Minori Abe[1], Tatsuya Suzuki[2], Yasuhiko Fujii[2], Masahiko Hada[1], [1]*Tokyo Metropolitan Universitiy, Japan,* [2]*Tokyo Institute of Technology, Japan*

PP036 **Towards Structure-Property-Function Relationships for Eumelanin**
B. J. Powell[1], A. Bernardus Mostert[1], Johannes de Boor[1], Seth Olsen[1], Jenny Riesz[3], Ian Gentle[2], Paul Meredith[1], [1]*Centre for Organic Photonics and Electronics, University of Queensland, Australia,* [2]*Department of Chemistry, University of Queensland, Australia,* [3]*Roam Consulting, Australia*

PP037 **Water's Optical Spectrum: Many-body Effects, Electrostatics and Coordination**
Andreas Hermann[1], Wolf Gero Schmidt[2], Peter Schwerdtfeger[1], [1]*New Zealand Institute for Advanced Study, Massey University, New Zealand,* [2]*Theoretische Physik, Universität Paderborn, Germany*

PP038 **The O of Rubisco: Oxygenase Reaction Mechanism and its Comparison with Rubisco Carboxylase Reactions**
Babu Kannappan[1], Jill Gready[1], [1]*John Curtin School of Medical Research, Australian National University, Australia*

PP039 **Studies of External Electric Field Effects on Chemical Reactivity and Stability**
Rahul Kar[1], K R S Chandrakumar[2], Sourav Pal[1], [1]*Physical Chemistry Division, National Chemical Laboratory, India,* [2]*Theoretical Chemistry Section, Bhabha Atomic Research Centre, India*

PP040 **Modelling Thiols on Au(111): A Possible Route to the SAM of SMMs. Structural, Thermodynamic, and Magnetic Properties of Simple Radicals.**
Bencini Alessandro[1], Gopalan Rajaraman[1], Federico Totti[1], Matteo Tusa[1], [1]*University of Florence, Department of Chemistry, Italy*

PP041 **Magnetic Interactions in Rare Earth Metal Nitronyl Nitroxide Chains**
Gopalan Rajaraman[1], Federico Totti[1], Alessandro Bencini[1], Andrea Caneschi[1], Roberta Sessoli[1], Dante Gatteschi[1], [1]*Università degli Studi di Firenze, Polo Scientifico, Dipartimento di Chimica, via della Lastruccia 3, Italy*

PP042 **Multidentate Ligands in Heterogeneous Ziegler-Natta Catalysts: A DFT Study**
Zygmunt Flisak[1], [1]*University of Opole, Institute of Chemistry, Poland*

Poster Session 1 – Sunday September 14 – 4.30-6.30pm

PP043 **Simple but Effective: Relativistic Pseudopotentials in Connection with Series of Correlation Consistent Basis Sets**
Detlev Figgen[1], Kirk A. Peterson[2], Hermann Stoll[3], [1]*New Zealand Institute for Advanced Study, Massey University, New Zealand,* [2]*Department of Chemistry, Washington State University, United States,* [3]*Institut für Theoretische Chemie, Universität Stuttgart, Germany*

PP044 **A Computational Approach to Study Toxin Binding to KcsA Potassium Channels**
Swarna Patra[1], Serdar Kuyucak[1], [1]*University of Sydney, School of Physics, Australia*

PP045 **Energy Landscape and Melting of Al_n Clusters and Nanoparticles**
Zhen Hua Li[1], Donald G. Truhlar[2], [1]*Department of Chemistry, Fudan University, China,* [2]*Department of Chemistry and Supercomputing Institute, University of Minnesota, United States*

PP046 **Quantum Monte Carlo Studies of the Chromium Dimer Cr_2**
Ryo Maezono[1], Michal Bajdich[2], Lubos Mitas[2], [1]*School of Information Science, JAIST, Japan,* [2]*Department of Physics, North Carolina State University, United States*

PP047 **A Hybrid QM/MM Study of the Z-FORMING® Metallosilicate Catalyst Based on Global and Local Descriptors in the Context of the HSAB Principle**
Rudy Coquet[1], Tsuyoshi Yamaguchi[1], Yuko Aoki[1], [1]*Nippon Oil Corporation, Japan*

PP048 **Are Carbodiphosphoranes Better Ligands than N-heterocyclic Carbenes for Grubb's Catalysts?**
Ralf Tonner[1], Gernot Frenking[2], [1]*Centre of Theoretical Chemistry and Physics (CTCP), New Zealand Institute for Advanced Study, Massey University, New Zealand,* [2]*Fachbereich Chemie, Philipps-Universität Marburg, Germany*

PP049 **Quantum Chemistry Component-Style**
Heather M. Netzloff[2], Teena Gulabani[3], Joseph P. Kenny[4], Curtis L. Janssen[4], Meng-Shiou Wu[3], Hirotoshi Mori[1], Masha Sosokina[3], Mark S. Gordon[1], Theresa L. Windus[1], [1]*Iowa State University, Department of Chemistry, United States,* [2]*US-DOE, Ames Laboratory, United States,* [3]*US-DOE, Ames Laboratory, Scalable Computing Laboratory, United States,* [4]*US-DOE, Sandia National Laboratory, Scalable Computing Research and Design, United States*

PP050 **Recent Algorithmic Development of Parallel Force Decomposition and Hamiltonian Splitting Methods for Macromolecular Simulation**
Urban Borštnik[1], Matej Praprotnik[1], Bernard R. Brooks[2], Dušanka Janežič[1], [1]*National Institute of Chemistry, Slovenia,* [2]*National Institutes of Health, United States*

PP051 **Do the Local Softness and Hardness Indicate the Softest and Hardest Region of a Molecule?**
Miquel Torrent-Sucarrat[1], Frank De Proft[1], Paul Geerlings[1], Paul W. Ayers[2], [1]*Vrije Universiteit Brussel (VUB), Eenheid Algemene Chemie (ALGC), Belgium,* [2]*McMaster University, Department of Chemistry, Canada*

PP052 **Local Softness and Hardness as Aromaticity Descriptors**
Miquel Torrent-Sucarrat[1], Paul Geerlings[1], [1]*Vrije Universiteit Brussel (VUB), Eenheid Algemene Chemie (ALGC), Belgium*

PP053 **Exploring the RGG box of Shadoo Using Molecular Dynamics**
Susan Corley[1], Jill Gready[1], [1]*Computational Proteomics and Drug Design Group, John Curtin School of Medical Research, Australian National Universty, Australia*

PP054 **Post-Hartree-Fock Methods and Dynamic Correlation in Atoms and Molecules**
Sergey Gusarov[1], Yurii Dmitriev[2], Tatiana Fedorova[2], Andriy Kovalenko[1], [1]*National Institute for Nanotechnology, Canada,* [2]*Fock Institute of Physics, Canada*

PP055 **Polarizabilities of Small Tin Clusters: Comparison between Theory and Experiment**
Behnam Assadollahzadeh[1], Peter Schwerdtfeger[1], [1]*Centre of Theoretical Chemistry and Physics/Institute for Advanced Studies (Massey University, Auckland), New Zealand*

PP056 **Ab Initio Calculations of Hydrogen Bond Free Energies: Developing a Model for Abraham's Solute Hydrogen Bond Donor Parameter**
J. Samuel Arey[1], Geoffrey P. F. Wood[2], [1]*Environmental Chemistry Modeling Laboratory, EPFL, Switzerland,* [2]*Laboratory of Computational Chemistry and Biochemistry, EPFL, Switzerland*

PP057 **Enhancing the Scope and Stereoselectivity of Umpolung Catalysis through Computational Techniques**
Kirsty Hawkes[1], Brian Yates[1], Tomislav Rovis[2], *[1]School of Chemistry, University of Tasmania, Australia, [2]Department of Chemistry, Colorado State University, United States*

PP058 **In-Vivo Protein Structure from Spectroscopy and Simulation**
Ben Corry[1], Annette Hurst[2], Boris Martinac[2], *[1]School of Biomedical, Biomolecular And Chemical Sciences, The University of Western Australia, Australia, [2]School of Biomedical Science, The University of Queensland, Australia*

PP059 **Circular Dichroism and Absorption Spectroscopy of Nucleosides with the SAC-CI Method**
Tomoo Miyahara[1], Hiroshi Sugiyama[3], Hiroshi Nakatsuji[3], *[1]Quantum Chemistry Research Institute, Japan, [2]JST CREST, Japan, [3]Kyoto University, Japan*

PP060 **Using a Black-Box Optimization Software to Determine the Second-Order Reduced Density Matrices of Atoms and Molecules by N-Representability Conditions**
Mituhiro Fukuda[1], Maho Nakata[2], Bastiaan J. Braams[3], Percus K. Jerome[4], Makoto Yamashita[5], Zhengji Zhao[6], Katsuki Fujisawa[7], *[1]Tokyo Institute of Technology, Global Edge Institute, Japan, [2]RIKEN, Advanced Center for Computing and Communication, Japan, [3]Emory University, Chemistry Department and Emerson Center for Scientific Computation, United States, [4]New York University, Department of Physics and Department of Mathematics, United States, [5]Kanagawa University, Department of Information Systems Creation, Japan, [6]Lawrence Berkeley National Laboratory, National Energy Research Scientific Computing Center, United States, [7]Chuo University, Department of Industrial and Systems Engineering, Japan*

PP061 **Improved Description of Polarization in Large Systems with Three-Layer ONIOM(QM:QM:MM)**
Marcus Lundberg[1], Yoko Sasakura[1], Guishan Zheng[2], Keiji Morokuma[1], *[1]Fukui Institute for Fundamental Chemistry, Kyoto University, Japan, [2]Department of Chemistry, University of Illinois at Urbana-Champaign, United States*

PP062 **On the Effect of Excess Electrons in Hexagonal Close-Packed Mg and Model Clusters**
Masae Takahashi[1], Mikio Fukuhara[1], Akihisa Inoue[1], Yoshiyuki Kawazoe[1], *[1]Institute of Materials Reseatch, Tohoku University, Japan*

PP063 **To be Advised**

PP064 **Ab Initio Studies of Lanthanide Trihalides by Means of Relativistic Model Core Potentials**
Shinya Tsukamoto[1], Hirotoshi Mori[2], Hiroshi Tatewaki[3], Eisaku Miyoshi[1], *[1]Graduate School of Engineering Sciences, Kyushu University, Japan, [2]Ocha-dai Academic Production Division of Advenced Sciences, Ochanomizu University, Japan, [3]Institute of Natural Sciences and Library and Information Processing Center, Nagoya City University, Japan*

PP065 **Solving the Schrödinger Equation of a Few Electron Atoms and Molecules Very Accurately with the Free ICI Method**
Hiroyuki Nakashima[1], Hiroshi Nakatsuji[1], *[1]Quantum Chemistry Research Institute, JST CREST, Japan; Kyoto University, Japan*

PP066 **Towards the Accurate Calculation of Enzymic Free Energy Surfaces: The Hydride-Ion Transfer in Dihydrofolate Reductase**
Peter Cummins[1], Ivan Rostov[1], Jill Gready[1], *[1]Computational Proteomics Group, John Curtin School of Medical Research, Australian National University, Australia*

PP067 **The Direct SAC-CI Method Applied to Molecular Potential Energy Surfaces**
Ryoichi Fukuda[1], Hiroshi Nakatsuji[1], *[1]Quantum Chemistry Research Institute, Japan; CREST, Japan, [3]Kyoto University, Japan*

PP068 **Study of Conformational States of ABC Exporters by Computer Modelling and Molecular Dynamics Simulations**
Jean-Paul Becker[1], Paul M. Tulkens[2], Françoise Van Bambeke[2], Martine Prévost[1], *[1]Université Libre de Bruxelles – Structure et Fonction des Membranes Biologiques, Belgium, [2]Université Catholique de Louvain - Unité de Pharmacologie Cellulaire et Moléculaire, Belgium*

PP069 **The Effect of Subsurface Rhenium on Chemisortion on Cobalt Surfaces: DFT Cluster Model Studies**
Ole Swang[1], Vebjørn Bakken[1], *[1]SINTEF Materials and Chemistry, Department of Hydrocarbon Process Chemistry, Norway*

Poster Session 1 – Sunday September 14 – 4.30-6.30pm

PP070 **Changes and Solvent Effects in the N1s, C1s and O1s Spectra of DNA/RNA Purine Bases with Respect to Unsubstituted Purine**
Quan Zhu[1], Feng Wang[1], Elena Ivanova[2], XiangYuan Li[3], *[1]Center for Molecular Simulation, Faculty of Information and Communication Technologies, Swinburne University of Technology, Australia, [2]Environment and Biotechnology Centre, Faculty of Life and Social Sciences, Swinburne University of Technology, Australia, [3]College of Chemical Engineering, Sichuan University, Chengdu, China*

PP071 **Atomic Description of Enzyme Catalysed Hydrogen Tunnelling: Two Case Studies**
Jiayun Pang[1], Nigel S. Scrutton[1], Michael J. Sutcliffe[1], *[1]Manchester Interdisciplinary Biocentre, University of Manchester, United Kingdom*

PP072 **Surficial Kirkwood-Buff Approach on the Analysis of the Preferential Exclusion Mechanism of Ectoine on the Protein Surface**
Isseki Yu[1], Masataka Nagaoka[1], *[1]Department of Information Science, Graduate School of Nagoya University, Japan*

PP073 **An Ab Initio-based Screening Tool for the Atmospheric Lifetimes of Iodine-Containing Species**
Florent Louis[1], Sébastien Canneaux[1], Jean-Francois Pauwels[1], Yi-Lei Zhao[2], Carlos Gonzalez[2], *[1]PC2A Université de Lille, France, [2]NIST, United States*

PP074 **A Theoretical Study of the Toluene and O-Xylene Oxidation**
Sébastien Canneaux[1], Florent Louis[1], Marc Ribaucour[1], Abderrahman El Bakali[1], Rodolphe Minetti[1], Jean-Francois Pauwels[1], *[1]PC2A Université de Lille, France*

PP075 **Estimation of the Thermokinetic Parameters for the Gas Phase {I-O-H} Reaction System Using Theoretical Chemistry**
Sébastien Canneaux[1], Florent Louis[1], Abderrahman El Bakali[1], Jean-François Pauwels[1], Bertrand Xerri[2], Laurent Cantrel[2], *[1]Universite des Sciences et Technologies de Lille, France, [2]IRSN, France*

PP076 **The Ultra-Violet Spectrum of $[Zn(pyridine)_4]^{2+}$**
Caroline Norris[1], Hazel Cox[1], *[1]University of Sussex, Department of Chemistry and Biochemistry, United Kingdom*

PP077 **Sparse Matrix Parallel Linear Algebra for Linear Scaling Quantum Chemical Calculations**
Urban Borštnik[1], Valéry Weber[1], Jürg Hutter[1], *[1]Physical Chemistry Institute, University of Zürich, Switzerland*

PP078 **Calculating Chemical Shifts and Charge Distributions of Biopolymers "On-The-Fly" – Structure Refinements using the Hybrid Force Field COSMOS-NMR**
Ulrich Sternberg[1], Raiker Witter[1], *[1]Karlsruhe Institute of Technology, Germany*

PP079 **Forming Concentric Double-Emulsion Droplets and Shells Using Electric Fields**
Alexander Tucker-Schwartz[1], Zongmin Bei[2], Robin L. Garrell[1], Thomas B. Jones[2], *[1]University of California, Los Angeles; Department of Chemistry & Biochemistry, United States, [2]University of Rochester; Department of Electrical & Computer Engineering, United States*

PP080 **Towards In-Silico Design of Antibiotics with Improved Permeation Properties**
Amit Kumar[1], Enrico Spiga[1], Francesca Collu[1], Eric Hajjar[1], Paolo Ruggerone[1], Matteo Ceccarelli[1], *[1]Dipartimento di Fisica, Universita di Cagliari, Italy*

PP081 **Computer Modeling of Structure and Dynamics of Photoactive Biotechnological Enzyme Nitrile Hydratase**
Wieslaw Nowak[1], Karina Kubiak[1], Lukasz Peplowski[1], *[1]Theoretical Molecular Biophysics Group, Institute of Physics, N. Copernicus University, Poland*

PP082 **The Photoisomerization of Fluorescent Protein Chromophores**
Seth Olsen[1], Ross McKenzie[1], *[1]Centre for Organic Photonics & Electronics and School of Physical Sciences, The University of Queensland, Australia*

PP083 **First-Principles Parameterisation of the Hubbard Model for Strongly-Correlated Half-Filled Layered Organic Semiconductors**
Edan Scriven[1], Ben Powell[1], *[1]School of Physical Sciences, University of Queensland, Australia*

PP084 **Calculated Electronic Transitions of the Water Ammonia Complex**
Joseph R. Lane[1], Veronica Vaida[2], Henrik G. Kjaergaard[1], [1]*Department of Chemistry, University of Otago, New Zealand,* [2]*Department of Chemistry and Biochemistry and CIRES, University of Colorado, United States*

PP085 **A QSAR Study for Predicting Aquatic Toxicity of Benzene Derivatives to Tetrahymena pyriformis**
Pornthip Boonsri[1], Waraporn Jungtanasombut[1], Supa Hannongbua[1], [1]*Department of Chemistry, Faculty of Science, Kasetsart University and Center of Nanotechnology Kasetsart University, and NANOTEC Center of Excellence at Kasetsart University, Thailand*

PP086 **DNA Molecular Recognition Pathways by Alkylating Agents: Insights from Molecular Dynamics**
Attilio Vittorio Vargiu[1], Paolo Ruggerone[1], Alessandra Magistrato[2], Paolo Carloni[1], [1]*University of Cagliari, Physics Department & SLACS, Italy,* [2]*SISSA/ISAS & DEMOCRITOS & IIT, Italy*

PP087 **The Hydrolysis Mechanism of the Anticancer Ruthenium Drugs NAMI-A and ICR Investigated by DFT–PCM Calculations**
Attilio Vittorio Vargiu[1], Arturo Robertazzi[2], Alessandra Magistrato[2], Paolo Ruggerone[1], Paolo Carloni[1], [1]*University of Cagliari, Department of Physics and Sardinian LAboratory for Computational Science (SLACS), Italy,* [2]*International School for Advances Studies (ISAS/SISSA)and DEMOCRITOS, Italy*

PP088 **Reaction of Nitrogen Oxides (NO_2, NO, N_2O) with ZnO Nanostructures for Gas Sensing Purposes: A DFT Study**
Michelle Spencer[1], Michael Breedon[1], Kester Wong[1], Irene Yarovsky[1], [1]*Applied Physics, RMIT University, Australia*

PP089 **The Reduced Density Matrix Method: Application of the T2' N-Representability Condition and Development of an Accurate Semidefinte Solver**
Maho Nakata[1], Bastiaan Braams[2], Katsuki Fujisawa[3], Mituhiro Fukuda[4], Jerome Percus[5], Makoto Yamashita[6], Zhengji Zhao[7], [1]*RIKEN, Advanced Center for Computing and Communication, Japan,* [2]*Emory University, Chemistry Department and Emerson Center for Scientific Computation, United States,* [3]*Chuo University, Department of Industrial and Systems Engineering, Japan,* [4]*Tokyo Institute of Technology, Global Edge Institute, Japan,* [5]*New York University, Courant Institute of Mathematical Sciences, United States,* [6]*Kanagawa University, Department of Information Systems Creation, Japan,* [7]*Lawrence Berkeley National Laboratory, National Energy Research Scientific Computing Center, Japan*

PP090 **Redox-Active Disulfide Bonds: A Quantum Chemical Approach**
Naomi Haworth[1], Jill Gready[2], Merridee Wouters[1], [1]*Computational Biology and Bioinformatics Program, Victor Chang Cardiac Research Institute, Australia,* [2]*Computational Proteomics Group, John Curtin School of Medical Research, Australia*

PP091 **A Viable Prebiotic Synthesis of Pantothenic Acid from Primeval Atmospheric Constituents**
Nigel Aylward[1], [1]*Queensland University of Technology, Physical and Chemical Sciences, Australia*

PP092 **Computational Study of Amyloid Fibril Like Peptide Aggregation**
Soonmin Jang[1], [1]*Sejong University, Korea, Republic of*

PP093 **Free Energy Based All-Atom Level Direct Folding Simulations of Mixed Folds**
Youngshang Pak[1], [1]*Department of Chemistry, Pusan National University, Korea, Republic of*

PP094 **Modelling Gas Adsorption in Metal Organic Frameworks**
Brad Wells[1], Zhijian Liang[1], Marc Marshall[1], Alan Chaffee[1], [1]*School of Chemistry, Monash University, Australia*

PP095 **Probing the Mobility of Hydrocarbons in Confined Systems through the Combined use of Molecular Modeling and Quasielastic Neutron Scattering**
M. Nguyen[1], K. W. Herwig[2], E. Kintzel[2], M. Kidder[3], P. Britt[3], A.C. Buchanan, III[3], A. L. Chaffee[1], [1]*School of Chemistry, Monash University, Australia,* [2]*Spallation Neutron Source, Oak Ridge National Laboratory, United States,* [3]*Chemical Sciences Division, Oak Ridge National Laboratory, United States*

PP096 **A New Linear Scaling Algorithm for Quantum-Chemical Calculations of Large Biomolecules**
Jian-Guo Yu[1], Wei-Hai Fang[1], Liang Peng[1], [1]*College of Chemistry Beijing Normal University, China*

Poster Session 1 – Sunday September 14 – 4.30-6.30pm

PP097 **Structure and Dynamics of Exopolysaccharides Produced by Inquilinus limosus, a New Pathogen of Cystic Fibrosis Patients**
Michelle Kuttel[1], Roberto Rizzo[2], Paula Cescutti[2], [1]*Department of Computer Science, University of Cape Town, South Africa,* [2]*Dipartimento di Biochimica Biofisica e Chimica delle Macromolecole, Università di Trieste, Italy*

PP098 **CO Adsorption and Dissociation on Hägg Fe Carbide Surfaces: Site Preference and the Role of Steps**
Melissa Petersen[1], Petrie Steynberg[1], Jan-Albert van den Berg[1], Werner Janse van Rensburg[1], [1]*Sasol Technology (Pty) Ltd, Research and Development Division, South Africa*

PP099 **Bulk and Surface Analysis of Hägg Fe-Carbide: A DFT Study**
Werner Janse van Rensburg[1], Jan-Albert van den Berg[1], Petrus J. Steynberg[1], [1]*Sasol Technology R&D, South Africa*

PP100 **Exploring the Reaction Mechanism of Cu-Catalysed Amine to Imine Oxidation**
Gemma Christian[1], Feliu Maseras[1], Antoni Llobet[1], Arnau Arbuse[2], M. Angeles Martinez[2], [1] *Institute of Chemical Research of Catalonia (ICIQ), Spain,* [2]*Departament de Química, Universitat de Girona, Spain*

PP101 **Ab Initio MD Methods for Free Energies of Chemical Reactions Coupled to Electron Transfer**
Yoshitaka Tateyama[1], Jochen Blumberger[3], Michiel Sprik[3], [1]*International Centre for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), Japan,* [2]*PRESTO, JST, Japan,* [3]*Department of Chemistry, University of Cambridge, United Kingdom*

PP102 **Probing Noncovalent Interactions in Biomolecular Crystals with Terahertz Spectroscopy**
Jörg Grunenberg[1], Thomas Kleine-Ostmann[1], Rafal Wilk[1], Martin Koch[1], Henning Niemann[1], Bernd Güttler[1], Kai Brandhorst[1], [1]*TU Braunschweig, Germany*

PP103 **Long Timescale Molecular Dynamics Simulations of Crystal Nucleation and Growth**
David Quigley[1], Mark Rodger[1], Colin Freeman[2], John Harding[2], [1]*Department of Chemistry / Centre for Scientific Computing, University of Warwick, United Kingdom,* [2]*Department of Engineering Materials, University of Sheffield, United Kingdom*

PP104 **Density Functional Theory Study of CO Oxidation on Pd Alloy Surfaces**
Michael Sullivan[1], Freda Lim[1], Jia Zhang[1], Hongmei Jin[1], Ping Wu[1], [1]*Institute of High Performance Computing, Singapore*

PP105 **Applicability of Two-Component Relativistic Theory Based on the Infinite-Order Foldy-Wouthuysen Transformation in Many-Electron Systems**
Junji Seino[1], Masahiko Hada[1], [1]*Tokyo Metropolitan University Department of Chemistry, Japan*

PP106 **A Theoretical Study of Fischer-Tropsch Reactions on FCC-Co(100)**
Jan-Albert van den Berg[1], Ionel Ciobica[1], Werner Janse van Rensburg[1], Petrus J Steynberg[1], [1]*Molecular Modelling; Sasol Technology, R & D, South Africa*

PP107 **Molecular Field Topology Analysis in Drug Design**
Vladimir Palyulin[1], Eugene Radchenko[1], Andrey Melnikov[1], Nikolay Zefirov[1], [1]*Department of Chemistry, M.V. Lomonosov Moscow State University, Russian Federation*

PP108 **Quantitative Description of Ring Conformations**
Vladimir Palyulin[1], Alexander Zotov[2], Sergey Pisarev[3], Nikolay Zefirov[1], [1]*Department of Chemistry, M.V. Lomonosov Moscow State University, Russian Federation,* [2]*N.D. Zelinsky Institute of Organic Chemistry RAS, Russian Federation,* [3]*Institute of Physiologically Active Compounds RAS, Russian Federation*

PP109 **Effects of Charge Reducing Mutations on Lysozyme Stability in Electromagnetic (e/m) Fields**
Gleb Solomentsev[1], Damian Mooney[1], Niall English[1], [1]*School of Chemical and Bioprocess Engineering University College of Dublin, Ireland*

PP110 **Azidolysis of Epoxides: Biocatalysis by Halohydrin Dehalogenase**
Dhurairajan Senthilnathan[1], Ponnambalam Venuvanalingam[1], [1]*School of Chemistry, Bharathidasan University, India*

PP111 **Global Properties from Localized States: Many-Electron Bands for Transition Metal Oxides**
Alexandrina Stoyanova[1], Coen de Graaf[2], Ria Broer[1], [1]*Zernike Institute for Advanced Materials, University of Groningen, Netherlands,* [2]*Universitat Rovira i Virgili, Spain*

PP112 **Effective Catalysis Employing Group II Metals**
Patricia Hunt[1], Andrew Sykes[1], [1]*Imperial College London, Chemistry Department, United Kingdom*

PP113 **Relativistic Quantum Chemistry to the Limits: Accuracy for the Small and Heavy**
Stefan Knecht[1], Lasse K. Sørensen[1], Hans Jørgen Aa. Jensen[2], Jeppe Olsen[3], Timo Fleig[1], [1]*Institute of Theoretical and Computational Chemistry, Heinrich Heine University Düsseldorf, Germany,* [2]*Department of Chemistry, University of Southern Denmark, Denmark,* [3]*Department of Chemistry, University of Aarhus, Denmark*

PP114 **A New Scale of Electronegativity Formulated in Terms of the Ionization Potentials of the Atoms**
Dulal Chandra Ghosh[1], [1]*Department of Chemistry, University of Kalyani, India*

PP115 **Natural Orbital Analysis of NMR Chemical Shifts of Cyanide Fe(III) Porphyrins and Cu(I) with Tridentate Ligands**
Daisuke Yamaki[1], Masanori Suzuki[1], Masahiko Hada[1], [1]*Department of Chemistry, Graduate School of Science, Tokyo Metropolitan University, Japan*

PP116 **Frequency Shifts in Rotational Spectra Caused by Parity Violating Effects**
Jürgen Stohner[1], Martin Quack[2], [1]*ZHAW Zürich University for Applied Sciences, Institute for Chemistry and Biological Chemistry, Switzerland,* [2]*ETH Zürich, Physical Chemistry, Switzerland*

PP117 **Energetic and Spectroscopic Properties of Polypeptides by Classical Molecular Dynamics : Relevance of a Second-Generation Force Field**
Carine Clavaguéra[1], David Semrouni[1], Gilles Ohanessian[1], [1]*Ecole Polytechnique / CNRS, France*

PP118 **Insight in Actinide Chemistry Through Computational Modeling and Gas-Phase Experiments**
Wibe de Jong[1], Gary Groenewold[2], Michael Van Stipdonk[3], [1]*Pacific Northwest National Laboratory, Environmental Molecular Sciences Laboratory, United States,* [2]*Idaho National Laboratory, Chemical Sciences, United States,* [3]*Wichita State University, Department of Chemistry, United States*

PP119 **An Intuitive Graphical User Interface for Quantum Chemical Simulations**
Jan Saam[1], John Stone[1], Klaus Schulten[1], [1]*Beckman Institute, University of Illinois, United States*

PP120 **Dynamic Oxygen Access Pathways in Proteins**
Jan Saam[2], Igor Ivanov[1], Matthias Walther[1], Hermann-Georg Holzhütter[1], Hartmut Kuhn[1], [1]*Charite - Universitaetsmedizin Berlin, Germany,* [2]*Beckman Institute, University of Illinois, United States*

PP121 **Interaction Energies of Histidine with Cations (H^+, Li^+, Na^+, K^+, Mg^{2+}, Ca^{2+})**
Saeedeh Hashemian[1], [1]*Azad University – Chemistry Department, Iran, Islamic Republic of*

PP122 **6-Electron 4-Centre Bonding: The Antiferromagnetism of Cu(II) Carboxylate Dimers**
Richard Harcourt[1], [1]*The University of Melbourne, Chemistry School, Australia*

PP123 **Modeling the Dehalogenation Step Catalyzed by Peroxidases**
Agnieszka Dybala-Defratyka[1], Michal Rostkowski[1], Piotr Paneth[1], [1]*Technical University of Lodz, Department of Chemistry, Poland*

PP124 **Trajectory Simulation of the Dynamics of Energy Transfer in the System CsBr + CsBr**
Vladimir Azriel[1], Lev Rusin[1], [1]*Institute of Energy Problems of Chemical Physics RAS, Russian Federation*

PP125 **Dynamics of Exchange Reaction in the Systems CsCl + RbI and CsBr + CsBr**
Vladimir Azriel[1], [1]*Institute of Energy Problems of Chemical Physics RAS, Russian Federation*

PP126 **The Effect of a Valley Bifurcation Point on a Potential Energy Surface and on Classical Dynamics**
Raúl Palmeiro[1], Obis Castaño[1], [1]*Dpto. de Química Física, Universidad de Alcalá, Spain*

PP127 **A Molecular Dynamics and QM/MM Study on the Catalytic Cycle of Acetohydroxyacid Synthase (AHAS)**
Gonzalo Jaña[1], Joel Alderete[1], Eduardo Delgado[1], Jordi Villà-Freixa[2], Xavier Prat-Resina[3], [1]*Universidad de Concepción & Theoretical and Computational Chemistry Group (QTC), Chile,* [2]*Barcelona Biomedical Research Park (PRBB) and Computational Biochemistry & Biophysics Lab (GRIB-IMIM/UPF), Spain,* [3]*University of Wisconsin & Department of Chemistry, United States*

Poster Session 1 – Sunday September 14 – 4.30-6.30pm

PP128 **Spectral Tuning of Human Visual Pigments Underlying Red, Green, and Blue Colour Vision**
Jun-Ya Hasegawa[1], Kazuhiro Fujimoto[1], Hiroshi Nakatsuji[2], [1]*Department of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University, Japan,* [2]*Quantum Chemistry Research Institute, Japan*

PP129 **Conformer-Selected Photodissociation: Ab Initio Multiple Spawning Dynamics of the Excited Propanal Cation**
Hongli Tao[1], Todd. J. Martínez[1], [1]*Department of Chemistry, University of Illinois, Urbana-Champaign, United States*

PP130 **Direct QM/MM Simulations of the Excited State Dynamics of Retinal Protonated Schiff Base in Isolation and in Complex Environments**
Chutintorn Punwong[1], Jane M. Owens[2], Todd J. Martínez[2], [1]*University of Illinois at Urbana-Champaign, Center for Biophysics and Computational Biology, United States,* [2]*University of Illinois at Urbana-Champaign, Department of Chemistry, United States*

PP131 **Inverse Gas Chromatographic Study of the Factors Affecting Surface Diffusivity of Gases Over Heterogeneous Solids**
Gavril Dimitrios[1], Rashid Atta Khan[1], [1]*University of Malaya, Malaysia*

PP132 **Comprehensive Reversible QSAR: Fragment Approach**
Kaido Tämm[1], [1]*University of Tartu, Estonia; Molcode Ltd., Estonia*

PP133 **Excited State Intramolecular Proton Transfer in 2-Aminopyridine and its Stacked Dimer as a Model System for the Excited-State Decay of Nucleic Acid Base Pairs**
Ashutosh Gupta[1], B.K. Mishra[2], N. Sathyamurthy[3], [1]*Department of Chemistry, Udai Pratap Autonomous College, India,* [2]*Department of Chemistry, Indian Institute of Technology, India,* [3]*Indian Institute of Science Education and Research, India*

PP134 **New Theoretical Tools for Determining the Structural Changes Enabling the Triplet Energy Transfer in Acceptor Molecules**
Luis Manuel Frutos[1], Obis Castaño[1], Ulises Acuña[1], [1]*University of Alcala, Departamento de Química Física, Spain; Instituto de Química Física "Rocasolano", C.S.I.C., Spain*

PP135 **Vibrational Spectroscopic Investigation and Theoretical Density Functional Theory (DFT) Calculations of 3-Piperidino-propylamine**
Mustafa Şenyel[1], Özgür Alver[1], Cemal Parlak[1], [1]*Anadolu University, Department of Physics, Turkey*

PP136 **FT-IR Spectroscopic Investigation of the Host–Guest Interactions in Some Hofmann Type Aniline Clathrates: M(1-Phenylpiperazine)$_2$Ni(CN)$_4$.C$_6$H$_5$NH$_2$ (M = Ni, Co and Cd)**
Mustafa Şenyel[1], Cemal Parlak[1], Özgür Alver[1], [1]*Anadolu University, Physics, Turkey*

PP137 **Characterization and Water Adsorption of Natural and Modified Sepiolite Having Dolomite From Turkey**
Burcu Erdoğan Alver[1], Meryem Sakizci[1], Ertugrul Yörükogullari[1], [1]*Anadolu University, Department of Physics, Turkey*

PP138 **Canonical Transformation for an Efficient Multireference Electronic Structure Method**
Takeshi Yanai[1], Eric Neuscamman[2], Garnet Chan[2], [1]*Institute for Molecular Science, Okazaki, Japan,* [2]*Cornell University, United States*

PP139 **Modelling Structural Properties of Bis(glycinato)copper(II) in Aqueous Solution**
Jasmina Sabolovic[1], [1]*Institute for Medical Research and Occupational Health, Croatia*

PP140 **Hydrogen Abstraction from CH_3OH and C_2H_5OH: A DFT, MP2, and CCSD(T) Study**
Orlando Roberto-Neto[1], Francisco B. C. Machado[1], Edson F. V. Carvalho[1], [1]*Instituto de Estudos Avançados, Brazil*

PP141 **Structure and Stability of (Ethanol)$_n$-Water, (n = 1, 2, and 3) Heterodimers, Heterotrimers, and Heterotetramers**
Sol Mejía[1], Juan Espinal[1], Fanor Mondragón[1], [1]*University of Antioquia, Colombia*

PP142 **Electronic States of XOONO (X = Cl, Br): Theoretical Studies**
Antonija Lesar[1], Milan Hodošček[2], [1]*Institute Jožef Stefan, Slovenia,* [2]*Natinal Institute of Chemistry, Slovenia*

PP143 **Dynamic Effects in Enzyme Catalysis. An Insight Using Grote-Hynes Theory**
Iñaki Tuñon[1], Javier J. Ruiz-Pernia[1], Vicent Moliner[2], James T. Hynes[3], Maite Roca[5], [1]*Departmento de Quimica Fisica, Universidad de Valencia, Spain,* [2]*Departamento de Quimica Fisica y Analitica, Universidad Jaume I, Spain,* [3]*Département de Chimie. Ecole Normale Supérieure., France,* [4]*Department of Chemistry and Biochemistry, University of Colorado, United States,* [5]*Department of Chemistry, University of Southern California, United States*

PP144 **Theoretical Calculations of Isotope Effects on Binding Oxamate to Lactate Dehydrogenase**
Katarzyna Swiderek[1], Artur Panczakiewicz[2], Grzegorz Bujacz[3], Piotr Paneth[1], [1]*Institute of Applied Radiation Chemistry, Technical University of Lodz, Poland,* [2]*FQS-Poland, Poland,* [3]*Institute of Technical Biochemistry, Faculty of Biotechnology and Food Sciences, Technical University of Lodz, Poland*

PP145 **Viscosity Kernels for Structured Molecular Fluids**
Ruslan Puscasu[1], Billy Todd[1], Peter Daivis[2], [1]*Swinburne University of Technology, Centre for Molecular Simulation, Australia,* [2]*RMIT University, Applied Physics, School of Applied Sciences, Australia*

PP146 **A Molecular Dynamic Study of Diffusion and Structure Properties of Carbon Dioxide in Water**
Tao Huang[1], Richard Sadus[1], [1]*Centre for Molecular Simulation, ICT, Swinburne University of Technology, Australia*

PP147 **Dinitrogen Activation in Three-Coordinate Transition Metal Complexes: A Molecular Orbital Rationalisation of Ligand Effects**
Alireza Ariafard[1], Nigel Brookes[1], Robert Stranger[1], Brian Yates[1], [1]*University of Tasmania & School of Chemistry, Australia*

PP148 **DFT Study of Reactions Between Hydrocarbons and Iodinating Agents**
Anna Yureva[1], Victor Filimonov[2], Oleg Poleshchuk[1], [1]*Tomsk State Pedagogical University, Russian Federation,* [2]*Tomsk Polytechnic University, Russian Federation*

PP149 **Electronic Structures and Chemical Indices of the Active Site of Oxygenated and Deoxygenated Hemerythrin**
Yu Takano[1], Kizashi Yamaguchi[2], Haruki Nakamura[1], [1]*Institution of Protein Research, Osaka University, Japan,* [2]*Center for Quantum Science and Technology under Extreme Conditions, Osaka University, Japan*

PP150 **^{1}H, ^{13}C, ^{15}N NMR and ^{n}J(C, H) Coupling Constants Investigation of 3-Piperidino-propylamine: A Combined Experimental and Theoretical Study**
Mustafa Şenyel[1], Özgür Alver[1], Cemal Parlak[1], [1]*Anadolu University, Department of Physics, Turkey*

PP151 **Dissociation Energies of Fluorocarbon-Substituted Donor-Acceptor Complexes**
Thomas Gilbert[1], Austin Gille[1], [1]*Northern Illinois University Department of Chemistry & Biochemistry, United States*

PP152 **Multiple Free Energies from a Single Simulation: Extending Enveloping Distribution Sampling to Nonoverlapping Phase-Space Distributions**
Clara D. Christ[1], Wilfred F. van Gunsteren[1], [1]*Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, Switzerland*

PP153 **Quantum Mechanical Study of Endo Cleavage Pathways in Anomerization of Glycosides**
Hiroko Satoh[1], Hans-Peter Lüthi[2], Jürg Hutter[3], Shino Manabe[4], [1]*Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, Switzerland,* [2]*National Institute of Informatics, Japan,* [3]*Institute of Physical Chemistry, University of Zürich, Switzerland,* [4]*RIKEN, The Institute of Physical and Chemical Research, Japan*

PP154 **Density Functional Studies of Aluminum Compounds in Aqueous Systems**
Jaakko Saukkoriipi[1], Kari Laasonen[1], [1]*University of Oulu, Department of Physical Chemistry, Finland*

PP155 **The Potentials of Mean Force for the Interaction of Hydrophilic Amino-Acid Side Chains in Water**
Mariusz Makowski[1], Adam Liwo[2], Harold A. Scheraga[2], [1]*University of Gdansk, Faculty of Chemistry, Poland,* [2]*Baker Laboratory of Chemistry and Chemical Biology, Cornell University, United States*

PP156 **Protolytic Equilibria in Methyl 3-Azido-6-iodo-2,3,6-trideoxy-α-D-arabino-Hexopyranoside Systems Studied by Ab Initio and Spectrophotometric Methods**
Aleksandra Dąbrowska[1], Mariusz Makowski[1], Dagmra Jacewicz[1], Agnieszka Chylewska[1], Lech Chmurzynski[1], [1]*University of Gdansk, Faculty of Chemistry, Poland*

Poster Session 1 – Sunday September 14 – 4.30-6.30pm

PP157 **An Improved Electronic Ground State Hessian for Use in TD-DFT Calculations**
Tom Ziegler[1], [1]*Department of Chemistry, University of Calgary, Canada*

PP158 **Toward Accurate Potentials for Condensed-Phase Chemical Reactions: Electrostatically Embedded Multi-Configuration Molecular Mechanics**
Masahiro Higashi[1], Donald G. Truhlar[1], [1]*Department of Chemistry and Supercomputing Institute, University of Minnesota, United States*

PP159 **Computational Determination of Equilibrium Constants for the Control Reaction of Nitroxide Mediated Polymerisation**
Jennifer Hodgson[1], Michelle Coote[1], [1]*ARC Centre of Excellence for Free Radical Chemistry and Biotechnology, Research School of Chemistry, Australian National University, Australia*

PP160 **Investigation of Natural Zeolites (Turkey) as a Desiccant**
Meryem Sakizci[1], Burcu Erdoğan Alver[1], Ertugrul Yörükoğullari[1], [1]*Anadolu University, Physics, Turkey*

PP161 **Conformational Analysis and Vibrational Assignment of 3-Phenylpropylamine**
Arslan Ünal[1], Mustafa Şenyel[1], Özgür Alver[1], Cemal Parlak[1], [1]*Anadolu University, Department of Physics, Science Faculty, Turkey*

PP162 **A Combined Experimental and Theoretical NMR Analyses of 3-Phenylpropylamine**
Özgür Alver[1], Arslan Ünal[1], Mustafa Şenyel[1], [1]*Anadolu University, Department of Physics, Science Faculty, Turkey*

PP163 **Reactions of 1-Naphthyl Radicals with Ethylene and Acetylene; Comparison of the Two Potential Energy Surfaces and the Two Kinetic Schemes**
Faina Dubnikova[1], Assa Lifshitz[1], [1]*The Hebrew University of Jerusalem, Israel*

PP164 **The Size and Site Dependence of Cation-π Interactions**
Dolly Vijay[1], G. Narahari Sastry[1], [1]*Molecular Modeling Group, Indian Institute of Chemical Technology, India*

PP165 **Cooperativity of Cation-π with Hydrogen Bonding and π-π Interactions: A Quantum Chemical Study**
Dolly Vijay[1], G. Narahari Sastry[1], [1]*Molecular Modeling Group, Indian Institute of Chemical Technology, India*

PP166 **Structural and Electronic Characteristics of Perhydrogenated CNTs and BNNTs**
Jukka Tanskanen[1], Mikko Linnolahti[1], Antti Karttunen[1], Tapani Pakkanen[1], [1]*University of Joensuu, Department of Chemistry, Finland*

PP167 **Calculation of Magnetically Induced Current Densities**
Dage Sundholm[1], Stefan Taubert[1], [1]*Department of Chemistry, University of Helsinki, Finland*

PP168 **Nitric Oxide Bonding to Heme Groups. Insight into Correlation in Fe(II) and Fe(III) Systems using Coupled Cluster Theory**
Julianna Olah[1], Jeremy N. Harvey[1], [1]*School of Chemistry, University of Bristol, United Kingdom*

PP169 **Metabolism of Dextromethorphan by Human CYP 2D6: A QM/MM Study**
Julianna Olah[1], Jeremy N. Harvey[1], [1]*School of Chemistry, University of Bristol, United Kingdom*

PP170 **Pushing the Limits of MCSCF**
Luke Roskop[1], Mark Gordon[1], [1]*Iowa State University Department of Chemistry, United States*

PP171 **Molecular Dynamics with Generalized Effective Fragment Potentials**
Jonathan Mullin[1], Mark Gordon[1], [1]*Iowa State University/Ames Laboratory, United States*

PP172 **Small Carbon Clusters Doped with First-Row Transition Metals: Structures and Stabilities**
Pilar Redondo[1], Carmen Barrientos[1], Laura Largo[1], Antonio Largo[1], [1]*Departamento de Química Física y Química Inorgánica, Universidad de Valladolid, Spain*

PP173 **Theory of Ultrafast Non–Resonant Multiphoton Transitions in Polyatomic Molecules: Basics and Application to Optimal Control Theory**
Markus Oppel[1], Volkhard May[2], Leticia González[3], David Ambrosek[4], [1]*Freie Universität Berlin - Fachbereich Biologie, Chemie, Pharmazie, Germany,* [2]*Humboldt Universität zu Berlin, Germany,* [3]*Friedrich-Schiller Universität Jena, Germany,* [4]*Université Louis Pasteur, France*

PP174 **MOGADOC - A Database with Experimental Gas-Phase Structures**
Jürgen Vogt[1], Natalja Vogt[1], [1]*Ulm University, Chemieinformationssysteme, Germany*

PP175 **Conformational Analysis of Some Biomolecules**
Natalja Vogt[1], [1]*Ulm University, Chemieinformationssysteme, Germany*

POSTER SESSION 2 – MONDAY SEPTEMBER 15 – 5.30-7.30pm

PP176 **Accurate N1s and C1s Core Electron Binding Energies for Substituted Pyridines Calculated by Density Functional Theory**
Yuji Takahata[1], Carl Wulfman[2], Delano Chong[3], [1]*State University of Campinas, Department of Chemistry, Brazil,* [2]*933 Strait View Drive, United States,* [3]*University of British Columbia, Department of Chemistry, Canada*

PP177 **Theoretical Methods for the Study of Reactions Involving Global Warming Gas Species Degradation and Byproduct Formation**
Hassan H. Abd Allah[1], Edet F. Archibong[2], Paul Blowers[3], Tony Ford[4], Rita Kakkar[5], Zhigang Shuai[6], Henry F. Schaefer III[7], Ponnadurai Ramasami[8], [1]*Baghdad University, Iraq,* [2]*University of Namibia, Namibia,* [3]*University of Arizona, United States,* [4]*University of Natal, South Africa,* [5]*University of Delhi, India,* [6]*Institute of Chemistry, China,* [7]*Centre of Computational Chemistry, United States,* [8]*University of Mauritius, Mauritius*

PP178 **Computational Study of the Substitution Effect on the Mechanism and Stereoselectivity of the Phospha-Wittig Reaction**
Hsin-Yi Liao[1], [1]*Department of Science Education, National Taipei University of Education, Taiwan*

PP179 **Quantum Interference: An Important Dimension for Manipulating Molecular Electron Transfer**
Gemma Solomon[1], David Andrews[1], Richard Van Duyne[1], Mark Ratner[1], [1]*Department of Chemistry, Northwestern University, United States*

PP180 **Computational Study of the Reactivity of Metal Cations with Methyl Fluoride**
Carmen Barrientos[1], Adrián Varela[2], Víctor M Rayón[1], Pilar Redondo[1], Laura Largo[1], Álvaro Cimas[3], José A Sordo[2], [1]*Universidad de Valladolid, Spain,* [2]*Universidad de Oviedo, Spain,* [3]*University d'Evry val d'Essonne, France*

PP181 **Modelling RAFT Polymerization Kinetics, a New Approach Based on Termination of Intermediates with Short Radicals**
Dominik Konkolewicz[1], Angus Gray-Weale[1], Sebastien Perrier[1], [11]*School of Chemistry, The University of Sydney, Australia*

PP182 **Are Dendrimers Like Randomly Branched Polymers?**
Dominik Konkolewicz[1], Angus Gray-Weale[1], [1]*School of Chemistry, University of Sydney, Australia*

PP183 **Polyhedral Allotropes of Phosphorus**
Antti Karttunen[1], Mikko Linnolahti[1], Tapani Pakkanen[1], [1]*University of Joensuu, Department of Chemistry, Finland*

PP184 **Theoretical Study of the Electron Transferase Activity of Cytochrome b5 Reductase**
Toshio Asada[1], Kichisuke Nishimoto[2], Shiro Koseki[1], [1]*Department of Chemistry, Faculty of Science, Osaka Prefecture University, Japan,* [2]*Department of Chemistry, Osaka City University, Japan*

PP185 **Interpretations of Raman and Raman Optical Activity Spectra of Flexible Acyclic Sugar Derivatives**
Jakub Kaminský[1], Josef Kapitán[1], Petr Bour[1], [1]*Institute of Organic Chemistry and Biochemistry, ASCR, Czech Republic*

PP186 **Ab Initio Calculations on the Orientation Dependence of the Na + CH_3NO_2 and CH_3NC Electron Transfer Reactions**
James Bull[1], Robert Maclagan[1], Peter Harland[1], [1]*Department of Chemistry, University of Canterbury, New Zealand*

PP187 **Theoretical Study on Azulenoids Containing Heavier Main Group Elements**
Yoshiaki Amatatsu[1], [1]*Faculty of Engineering and Resource Science, Akita University, Japan*

PP188 **Computational Study of the Solvent Effect upon the Interaction Between the Guanidinium Cation and Aromatic Systems**
Enrique M. Cabaleiro-Lago[1], Jesús Rodríguez-Otero[2], Ángeles Peña-Gallego[2], [1]*Departamento de Química Física, Facultade de Ciencias, Universidade de Santiago de Compostel, Spain,* [2]*Departamento de Química Física, Facultade de Química, Universidade de Santiago de Compostela, Spain*

PP189 **Theoretical Study of the Solvent Effect on the Interaction between the Pyridinium Cation and Benzene**
Jesús Rodríquez-Otero[1], Enrique M. Cabaleiro-Lago[2], Angeles Pena-Gallego[1], [1]*Universidade de Santiago de Compostela, Departamento de Quimica Fisica, Spain,* [2]*Universidade de Santiago de Compostela, Departamento de Quimica Fisica, Spain*

PP190 **Benchmark Calculations of the Nuclear Electric Quadrupole Moment in Heavy Atomic Systems**
Ephraim Eliav[1], Hanna Yakobi[1], Igor Itkin[1], Uzi Kaldor[1], [1]*Chemistry School, Tel Aviv University, Israel*

PP191 **Dynamic Quantum Isotope Effects on Multiple Proton Transfer Reactions**
Yasuteru Shigeta[1,2], [1]*Department of Physics, Tsukuba University, Japan,* [2]*Institute of Picobiology, University of Hyogo, Japan*

PP192 **Characteristics of the Vertical (Pd…Solvent) Interaction at the First Solvation Shell of the Square Planar Pd Complexes**
Jong Keun Park[1], [1]*Department of Chemistry Education, Research Institute of Natural Science, and Educational Research Institute, Gyeongsang National University, Korea, Republic of*

PP193 **Perturbation Expansions Based on Absolutely Local Excited Molecular Orbitals**
Suehiro Iwata[1], [1]*Toyota Physical and Chemical Research Institute, Japan*

PP194 **Theoretical Study of First-Row Transition Metal Dimers using Newly Developed spdsMCP**
Ma San Mon[1], Hirotoshi Mori[1], Eisaku Miyoshi[1], [1]*Interdisciplinary Graduate School of Engineering Science, Kyushu University, Japan*

PP195 **Automatically Generated Coulomb-Fitting Basis Sets: Design and Accuracy for Systems Containing H to Kr**
Rui Yang[1], Alistair Rendell[1], Michael Frisch[2], [1]*Department of Computer Science, ANU College of Engineering and Computer Science, The Australian National University, Australia,* [2]*Gaussian Inc., United States*

PP196 **Vibrational Raman Optical Activity Spectra of Chiral Metal Complexes**
Sandra Luber[1], Markus Reiher[1], [1]*Swiss Federal Institute of Technology Zürich, Laboratory of Physical Chemistry, Switzerland*

PP197 **A New Algorithm for Energy Gradients and Orbital Optimization in the Non-Orthogonal Valence Bond Method**
Lingchun Song[1], Jinshuai Song[1], Yirong Mo[1], Wei Wu[1], [1]*Department of Chemistry, Xiamen University, China*

PP198 **Ab Initio Fragment Molecular Orbital Study of Molecular Interactions in Liganded Retinoid X Receptor: Specification of Residues Associated with Ligand Inducible Information Transmission**
Mika Ito[1], Kaori Fukuzawa[2], Takeshi Ishikawa[3], Yuji Mochizuki[4], Tatsuya Nakano[5], Shigenori Tanaka[6], [1]*Karolinska Institute, Sweden,* [2]*Mizuho Information and Research Institute, Inc., Japan,* [3]*Gifu University, CEID, Japan,* [4]*Rikkyo University, Department of Chemistry, Faculty of Science, Japan,* [5]*National Institute of Health Sciences, Division of Medicinal Safety Science, Japan,* [6]*Kobe University, Graduate School of Human Development and Environment, Japan*

PP199 **Generating Benchmark Interaction Energies for Weakly Bound Non-Covalent Clusters with the 2-Body:Many-Body Multicentered QM:QM Method**
Desiree Bates[1], Gregory Tschumper[1], [1]*University of Mississippi, Department of Chemistry and Biochemistry, United States*

PP200 **Structural and Dynamical Properties of Myoglobins Probed by Molecular Dynamics Simulations**
Andrea Scorciapino[1], Enrico Spiga[2], Mariano Casu[2], Paolo Ruggerone[1], Matteo Ceccarelli[1], [1]*Department of Physics, University of Cagliari, Italy,* [2]*Department of Chemistry, University of Cagliari, Italy*

PP201 **Determination of the Atom Transfer Radical Polymerisation Mechanism**
Ching Yeh Lin[1], Michelle Coote[1], Armando Gennaro[2], Krzysztof Matyjaszewski[3], [1]*Research School of Chemistry, ANU, Australia,* [2]*Università di Padova, Italy,* [3]*Carnegie Mellon University, United States*

PP202 **Site Specificity of the $^{\alpha}$C-H bond Dissociation Energy for a Naturally Occurring β-Hairpin Peptide - An Ab Initio Study**
Ren-Jie Lin[1], Wan-Chun Cheng[1], Feng-Yin Li[1], [1]*Department of Chemistry of National Chung Hsing University, Taiwan*

Poster Session 2 – Monday September 15 – 5.30-7.30pm

PP203 **A QM/MM Study of the Thymidylate Synthase Molecular Mechanism**
Natal Kanaan[1], Vicent Moliner[1], Sergio Martí[1], [1]*Universitat Jaume I, Departament de Química Física i Analítica, Spain*

PP204 **Theoretical Approaches to the Feasibility of the Ribocell Model**
Pier Luigi Della Gatta[1], Fabio Mavelli[1], Pier Luigi Luisi[2], [1]*Chemistry Department - University of Bari, Italy,* [2]*Biology Department, University of Roma Tre, Italy*

PP205 **An Ab Initio Structural Study of Dithiol Adsorption on Au(111)**
Fulvio Ciriaco[1], Savio Laricchia[1], Fabio Mavelli[1], Luigi Cassidei[1], [1]*Chemistry Department - University of Bari, Italy*

PP206 **The Full Explicitly-Correlated Coupled-Cluster Method with Single and Double Excitations**
Toru Shiozaki[1,2], Muneaki Kamiya[1], So Hirata[1], Edward F. Valeev[3], [1]*Quantum Theory Project, Department of Chemistry and Department of Physics, University of Florida, United States,* [2]*Department of Applied Chemistry, Graduate School of Engineering, The University of Tokyo, Japan,* [3]*Department of Chemistry, Virginia Tech, United States*

PP207 **Distortion/Interaction Analysis of the Reactions of Small Rings**
Elizabeth Krenske[1], K. N. Houk[1], [1]*University of California, Los Angeles, Department of Chemistry and Biochemistry, United States*

PP208 **Computational Studies on Electron and Proton Transfer between Phenol-Imidazole-Base Triads**
Lee Jin Yong[1], Kang Sunwoo[1], Yan Shihai[1], Ko Kyung Chul[1], [1] *Department of Chemistry, Sungkyunkwan University, Korea, Republic of*

PP209 **A Rationally Designed Fluorescence 'Turn-On' Cu^{2+} Sensor and 'Turn-On' α-Amino-Carboxylate Sensor**
Kyoung Chul Ko[1], Shihai Yan[1], Sunwoo Kang[1], Jin Yong Lee[1], [1]*Department of Chemistry, Sungkyunkwan University, Korea, Republic of*

PP210 **Evidence for β-Elimination Explains the Regioselectivity in the Rh-Catalyzed Hydroformylation of Vinylidenic Substrates**
Giuliano Alagona[1], Caterina Ghio[1], [1]*CNR-IPCF-MML, Italy*

PP211 **Secondary and Tertiary Rh-Alkyl Intermediate Competition in the Hydroformylation of 1-Methylcyclohexenes and Related Linear Olefins**
Giuliano Alagona[1], Caterina Ghio[1], Raffaello Lazzaroni[2], [1]*CNR-IPCF-MML, Italy,* [2]*Univ. of Pisa-DCCI, Italy*

PP212 **Chemical Bonding in the Lightest Tri-Atomic Clusters; H_3^+, Li_3^+ and B_3^-**
Cina Foroutan-Nejad[1], Parviz Rashidi-Ranjbar[1], [1]*Department of Chemistry, University of Tehran, Iran, Islamic Republic of*

PP213 **Assessing σ-Aromaticity by Studying One-Electron Density–NICS Relationships**
Cina Foroutan-Nejad[1], [1]*Department of Chemistry, University of Tehran, Iran, Islamic Republic of*

PP214 **The Role of Hydrogen Bonds and Cation-Bridges on the Thermodynamic Stability of Humic Acids: Modeling Study**
Adelia Aquino[1], Daniel Tunega[2], Hasan Pasalic[1], Georg Haberhauer[3], Martin Gerzabek[2], Hans Lischka[1], [1]*University of Vienna/Institute for Theoretical Chemistry, Austria,* [2]*University of Natural Resources and Applied Life Sciences Vienna, Austria,* [3]*Austrian Research Centres, Seibersdorf, Austria*

PP215 **Xenon NMR in Single-Wall Carbon Nanotubes: Dependence of the Chemical Shift on the Adsorption Site and Tube Type**
Perttu Lantto[1], Juha Vaara[2], [1]*University of Oulu, Department of Physical Sciences, Finland,* [2]*University of Helsinki, Department of Chemistry, Finland*

PP216 **Oxygen Radical-Mediated Oxidation Reactions of a Simple Peptide Motif – An Ab Initio Study**
Jui-Chuan Chang[1], Feng-Yin Li[1], [1]*Department of Chemistry, National Chung Hsing University, Taiwan*

PP217 **Local Aromaticity of Graphene and its Electron Transport Properties**
You-Cheng Chan[1], Fu-Der Mai[2], Hong-Yi Tang[3], Feng-Yin Li[1], [1]*Department of Chemistry, National Chung Hsing University, Taiwan,* [2]*Department of Biochemistry, School of Medicine, Taipei Medical University, Taiwan,* [3]*Department of Applied Chemistry, National Chi Nan University, Taiwan*

PP218 **Ion-Pair Binding Energies in Ionic Liquids: Relationship to Physical Properties**
Uditha Bernard[1], Ekaterina Izgorodina[1], Douglas MacFarlane[1], [1]*School of Chemistry, Monash University, Australia*

PP219 **Theoretical Elucidation of the Antioxidant Mechanism of 1,3-Dihydro-1-methyl-2H-imidazole-2-selenol (MSeI)**
Soujanya Yarasi[1], Garikapati Narahari Sastry[1], [1]*Molecular Modeling Group, Indian Institute of Chemical Technology, India*

PP220 **Theoretical Study on the Hydrated Structures of Y^{3+} and La^{3+} Using Model Core Potentials**
Takayuki Fujiwara[1], Hirotoshi Mori[2], Hiroshi Tatewaki[3], Eisaku Miyoshi[1], [1]*Graduate School of Engineering Sciences Kyushu University, Japan,* [2]*Ocha-dai Academic Production Ochanomizu University, Japan,* [3]*Graduate School of Natural Sciences and Information Center, Nagoya City University, Japan*

PP221 **Design for Spintronics Materials: Comparison of Electronic States of X_2YSi (X, Y = Mn, Fe, Co) Thin Films**
Yohsuke Odahara[1], Daisuke Shigyo[2], Hirotoshi Mori[3], Tsuyoshi Yoshitake[1], Eisaku Miyoshi[1], [1]*Graduate School of Engineering Sciences Kyushu University, Japan,* [2]*Toyo Kohan Co. Ltd., Japan,* [3]*Ocha-dai Academic Production Ochanomizu University, Japan*

PP222 **Theoretical Study of Intermolecular Interactions using the Model Core Potential (MCP)**
Yasunori Yamashita[1], Hirotoshi Mori[2], Eisaku Miyoshi[1], [1]*Graduate School of Engineering Sciences Kyushu University, Japan,* [2]*Ocha-dai Academic Production Ochanomizu University, Japan*

PP223 **A Theoretical Study of Organic Benzothiadiazole Based Dyes for Dye Sensitized Solar Cells**
Adrian Mak[1], Michael Sullivan[1], [1]*Institute of High Performance Computing, Singapore*

PP224 **Hybrid Ab Initio Valence Bond / Molecular Mechanics (VB/MM), A New Method for Calculating Biochemical Systems**
Avital Shurki[1], Hadar Crown[1], Tamar Shnerb[1], Avital Sharir-Ivry[1], [1]*Department of Medicinal Chemistry and Natural Products, School of Pharmacy The Lise Meitner-Minerva Center for Computational Quantum Chemistry The Hebrew University of Jerusalem, Israel*

PP225 **DNA Recombinase Protein of the Mycobacterium tuberculosis, its Function and Structure, a Computational Study**
Claudio Carra[1], Francis A. Cucinotta[1], [1]*USRA-NASA/JSC, United States*

PP226 **Theoretical Investigations of Lanthanoid Carboxylates: 'Green' Corrosion Inhibitors**
Rebecca Abramson[1], Peter Junk[1], Glen Deacon[1], Ekaterina Izgorodina[1], Kim Baldridge[2], [1]*Monash University, School of Chemistry, Australia,* [2]*University of Zürich, Organic Chemistry Institute, Switzerland*

PP227 **Structures of Complexes of Ru(III) and Pd(II) with 3-(2'-Thiazolylazo)-2,6-diaminopyridine: a DFT Study**
Ratanon Chotima[1], Apisit Songsasen[1], Waraporn Parasuk[1], [1]*Department of Chemistry, Kasetsart University, Thailand*

PP228 **Xenoreactive Antibodies: Structural Key to Overcoming Rejection**
Mark Agosting[1], James Swarbrick[1], Phil Thompson[1], Mauro Sandrin[3], Paul Ramsland[2], Elizabeth Yuriev[1], [1]*Victorian College of Pharmacy, Department of Medicinal Chemsitry, Australia,* [2]*Burnet Institute, Australia,* [3]*The University of Melbourne, Department of Surgery, Austin and Northern Health, Australia*

PP229 **Activation and Scission of CO_2 using Three Coordinate d_2 Transition Metal Complexes. A DFT Study**
Nigel Brookes[1], Brian Yates[1], Robert Stranger[1], [1]*University of Tasmania, Chemistry Department, Australia*

PP230 **Substituent Effects on α-Carbon Acidities – A Combined Theoretical and Experimental Investigation**
Junming Ho[1], Satish Chand[1], Christopher Easton[1], Michelle Coote[1], [1]*ARC Centre of Excellence in Free Radical Chemistry and Biotechnology, Research School of Chemistry, Australian National University, Australia*

PP231 **Linear-Scaling Correlated Quantum Chemical Calculations with the Divide-and-Conquer Method**
Masato Kobayashi[1], Hiromi Nakai[1], [1]*Department of Chemistry and Biochemistry, School of Advanced Science and Engineering, Waseda University, Japan*

Poster Session 2 – Monday September 15 – 5.30-7.30pm

PP232 **Reaction Field Effects on the Nitrile Bond in Acetonitrile, Benzonitrile, Hydrogen Cyanide and t-Butyl Cyanide**
Feryal Safinejad[1], Mehdi Asghari-Khiavi[1], [1]*School of Chemistry, Monash University, Australia*

PP233 **Molecular Dynamics Simulation of a Thin Oxygen Film Covering the Fullerene C_{60}**
Mehdi Asghari-Khiavi[1], Feryal Safinejad[1], [1]*School of Chemistry, Monash University, Australia*

PP234 **[4+2] Cycloadditions of 2- and 3-Vinyl Cyclic and Heterocyclic Systems and Maleic Anhydride: A Theoretical Analysis**
G. Narahari Sastry[1], Gaddamanugu Gayatri[1], [1]*Indian Institute of Chemical Technology & Molecular Modeling Group, India*

PP235 **Ab Initio Path Integral Molecular Dynamics using the ONIOM Method**
Motoyuki Shiga[1], [1]*Japan Atomic Energy Agency, Japan*

PP236 **Copper Binding Site and Redox Chemistry of the Amyloid-β Protein in Alzheimer's Disease**
Vidana Epa[1], Victor Streltsov[1], Stephen Titmuss[1], Jose Varghese[1], [1]*CSIRO Molecular Health & Technologies, Australia*

PP237 **Theoretical Study of the Dioxygen Activation Mechanism in Iron(III) Catechol Dioxygenase: "Oxygen Activation" vs. "Substrate Activation"**
Naoki Nakatani[1], Yoshihide Nakao[1], Hirofumi Sato[1], Shigeyoshi Sakaki[1], [1]*Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, Japan*

PP238 **Unusual π-Type Interactions Between the Chelated Cu(II) Cation and the C=C Bond in the Vitamin B_{13} Complex: A Theoretical Study**
Rafal Wysokinski[1], Katarzyna Hernik[1], Wiktor Zierkiewicz[1], Danuta Michalska[1], [1]*Wroclaw University of Technology, Faculty of Chemistry, Poland*

PP239 **Silabutadienes: Internal Rotations and π–Conjugation – A DFT Study**
Hong-Wei Xi[1], Miriam Karni[1], Yitzhak Apeloig[1], [1]*Schulich Faculty of Chemistry and the Lise Meitner - Minerva Center for Computational Quantum Chemistry, Technion-Israel Institute of Technology, Israel*

PP240 **Magnetic Properties of $Sc_3C_2@C_{80}$ Including Dynamical Effects**
Stefan Taubert[1], Michal Straka[2], Teemu O. Pennanen[1], Dage Sundholm[1], Juha Vaara[1], [1]*University of Helsinki, Department of Chemistry, Finland,* [2]*Academy of Sciences of the Czech Republic, Institute of Org. Chemistry and Biochemistry, Czech Republic*

PP241 **A Computational Study of the Oxygen Evolving Mn_2-Dimeric Porphyrin Complex: Implications for the Catalytic Oxidation of Water**
W. M. C. Sameera[1], John E. McGrady[1], [1]*WestCHEM and the Department of Chemistry, University of Glasgow, United Kingdom*

PP242 **Accurate Quartic Force Fields for CCH^- and NH_2^-**
Xinchuan Huang[1], David Schwenke[1], Timothy Lee[1], [1]*NASA Ames Research Center, United States*

PP243 **Theoretical Study of the Deprotonation of Fluorine-Substituted Benzenes**
Mansoor Namazian[1], Michelle Coote[1], [1]*Research School of Chemistry, Australian National University, Australia*

PP244 **A DFT Study on the Catalytic Mechanism of a DNA/RNA Repair Enzyme AlkB**
Haining Liu[1], James W. Gauld[1], [1]*Department of Chemistry and Biochemistry, University of Windsor, Canada*

PP245 **Theoretical Studies of Metallo (Li and Na) – Ene Reaction Mechanisms**
Shogo Sakai[1], Takahiro Hikida[1], [1]*Gifu University, Japan*

PP246 **Acetone, Acetaldehyde and Acetophenone on the Si(001) Surface: Atomic Scale Images and First Principle Calculations**
Daniel Belcher[1], Steven Schofield[2], Philip Smith[1], Marian Radny[1], Oliver Warschkow[3], Sherin Saraireh[4], [1]*The University of Newcastle, School of Mathematical and Physical Sciences, Australia,* [2]*University College London, London Centre for Nanotechnology, United Kingdom,* [3]*The University of Sydney, Centre for Quantum Computer Technology, Australia,* [4]*Bin Talal University, Department of Physics, Jordan*

PP247 **An NMR-DFT Study of Arsenicin A, the First Polyarsenical from Nature**
Petri Tähtinen[1], Giacomo Saielli[2], Graziano Guella[3], Ines Mancini[3], Alessandro Bagno[2], [1]*University of Turku, Department of Chemistry, Finland,* [2]*University of Padova, Department of Chemistry, Italy,* [3]*University of Trento, Department of Physics, Italy*

PP248 **Dynamics of Isomerization of Cyclohexadiene to Hexatriene and Laser Control of the Dynamics**
Hiroyuki Tamura[1], Shinkoh Nanbu[2], Toshimasa Ishida[3], Hiroki Nakamura[1], [1]*Institute for Molecular Science, Japan,* [2]*Research Institute for Information Technology, Kyushu University, Japan,* [3]*Fukui Institute for Fundamental Chemistry, Kyoto University, Japan*

PP249 **Oxidation of Cyclohexane by a High-Valent Iron Bispidine Complex – A Combined Experimental and Computational Study**
Prabha Vadivelu[1], Martin Maurer[1], Peter Comba[1], [1]*Universität Heidelberg, Anorganisch-Chemisches Institut, Germany*

PP250 **An Investigation of Intermolecular Addition Involving Acetyl and Fluoroacyl Radicals**
Tu Anh Tran[1], Carl Schiesser[1], [1]*School of Chemistry, Bio21 Molecular Science and Biotechnology Institute, The University of Melbourne, Australia*

PP251 **Ab Initio Calculations of Single Electron Capture in Proton – Water Molecule Collisions at Low and Intermediate Energies**
Pablo Martinez[1], Luis Fernando Errea[1], Luis Mendez[1], Ismanuel Rabadan[1], Clara Illescas[1], [1]*Universidad Autonoma de Madrid, Departamento de Quimica, Spain*

PP252 **The Mechanism of $B(C_6F_5)_3$-Catalyzed Hydrogenation of Imines**
Andrea Hamza[1], András Stirling[1], Tibor András Rokob[1], Imre Pápai[1], [1]*Chemical Research Center of HAS, Hungary*

PP253 **Theoretical Investigations on the Relative Stability of Niobium Compounds**
Eduardo Cassús[1], Wladmir de Souza[1], Ana Carlota dos Santos[1], [1]*PETROBRAS/CENPES, Brazil*

PP254 **Theoretical Study of Degradation Reactions of Alkanes (C2-C4) in the ZSM-5 Zeolite**
Kanjarat Sukrat[1], Vudhichai Parasuk[1], Daniel Tunega[2], Adelia Aquino[3], Hans Lischka[2], [1]*Department of Chemistry, Faculty of Science, Chulalongkorn University, Thailand,* [2]*Institute for Theoretical Chemistry University of Vienna Währingerstrasse 17, A-1090, Austria,* [3]*Institute of Soil Research, University of Natural Resources and Applied Life Sciences, Peter-Jordan-Strasse 82, A-1190, Austria*

PP255 **Efficient Self-Consistent-Field Solution for the Nondynamical Correlation Functional**
Jing Kong[1], Emil Proynov[1], Yihan Shao[1], [1]*Q-Chem Inc., United States*

PP256 **A QM/MM Investigation of the Catalytic Mechanism of Coenzyme B_{12}- Independent Glycerol Dehydratase (GDH)**
Borislav Kovacevic[1], Gregory M. Sandala[2], Leo Radom[2], David M. Smith[1], [1]*Rudjer Boškovic Institute, Department of Organic Chemistry and Biochemistry, Croatia,* [2]*The University of Sydney, School of Chemistry, Australia*

PP257 **Molecular Dynamics Studies of the Hydrophobin EAS at Air:Water Interfaces**
Itamar Kass[1], Rima Gupte[1], Alan Mark[1], [1]*The University of Queensland, School of Molecular and Microbial Sciences, Australia*

PP258 **Theoretical Investigations on the Structural and Energetic Properties of Low-Lying Electronic States of Thiophenol**
Heechol Choi[1], Yoon Sup Lee[1], [1]*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea, Republic of*

PP259 **Wetting of Nanostructured Polymer Surfaces**
Janne Hirvi[1], Tapani Pakkanen[1], [1]*University of Joensuu, Department of Chemistry, Finland*

PP260 **Continuous Symmetry Analysis of the Cis-Trans Isomerizations of Diazene Derivatives: The Symmetry Transition Point**
Inbal Tuvi-Arad[1], David Avnir[2], [1]*Department of Natural Sciences, The Open University of Israel, Israel,* [2]*Institute of Chemistry, The Hebrew University, Israel*

Poster Session 2 – Monday September 15 – 5.30-7.30pm

PP261 **Density Functional Description of Quantum Transport and its Application to Single-Molecule Conductance**
Sören Wohlthat[1], Fabian Pauly[2,3], Jeffrey R. Reimers[1], [1]*School of Chemistry, The University of Sydney, Australia,* [2]*Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures, Universität Karlsruhe, Germany,* [3]*Institut für Nanotechnologie, Forschungszentrum Karlsruhe, Germany*

PP262 **Conformational Changes of A-RNA and A′-RNA by Unrestrained Molecular Dynamic (MD) Simulation in Aqueous Solution**
Defang Ouyang[1], Hong Zhang[2], Harendra Parekh[1], Sean Smith[2], [1]*School of Pharmacy, The University of Queensland, Australia,* [2]*Centre for Computational Molecular Science, Australian Institute of Bioengineering and Nanotechnology, The University of Queensland, Australia*

PP263 **Adsorption State and Behavior of Small Molecules in Nanochanneled Metal-Organic Frameworks: An Electronic State Calculation**
Yusuke Ohta[1], Haruko Hitomi[1], Masataka Nagaoka[1], [1]*Department of Complex Systems Science, Graduate School of Information Science, Nagoya University, Japan*

PP264 **Microscopic Hydration Mechanism in the Ammonia Dissolution Process: Importance of the Solute QM Polarization**
Norio Takenaka[1], Yoshiyuki Koyano[1], Masataka Nagaoka[1], [1]*Department of Complex Systems Science, Graduate School of Information Science, Nagoya University, Japan*

PP265 **Theoretical Study on Isotope Effects in Polypeptides Based on Path Integral Molecular Dynamics and Fragment Molecular Orbital Methods**
Takatoshi Fujita[1], Hirofumi Watanabe[2], Shigenori Tanaka[1], [1]*Graduate School of Human Development and Environment, Kobe University, Japan,* [2]*CREST, Japan Science and Technology Agency, Japan*

PP266 **Implementation of the MP2 Gradient in the Generalized Hybrid Orbital (GHO) Method**
Jaewoon Jung[1], Seiichiro Ten-no[1], [1]*Graduate School of Information Science, Nagoya University, Japan*

PP267 **Theoretical Study of the Excited States of DsRed Mutants by the Fragment Molecular Orbital Method**
Naoki Taguchi[1], Yuji Mochizuki[1], Tatsuya Nakano[2], Takeshi Ishikawa[3], Kaori Fukuzawa[4], Minoru Sakurai[5], Shigenori Tanaka[6], [1]*Department of Chemistry, Faculty of Science, Rikkyo University, Japan,* [2]*Division of Safety Information on Drug, Food and Chemicals, National Institute of Health Sciences, Japan,* [3]*Division of Prion Research, Center for Emerging Infectious Diseases, Gifu University, Japan,* [4]*Mizuho Information & Research Institute Inc., Japan,* [5]*Center for Biological Resources and Informatics, Tokyo Institute of Technology, Japan,* [6]*Graduate School of Science and Technology, Kobe University, Japan*

PP268 **DFT Errors in Organic Reactions**
David Brittain[1], Ching Yeh Lin[1], Andrew Gilbert[1], Ekaterina Izgorodina[3], Peter Gill[1], Michelle Coote[1,2] [1]*Research School of Chemistry, Australian National University, Australia,* [2]*ARC Centre of Excellence in Free Radical Chemistry and Biotechnology, Australia,* [3]*School of Chemistry, Monash University, Australia*

PP269 **The CCSD(T)-F12 Method Using the Hybrid QD/RI Approach**
Denis Bokhan[1], Seiichiro Ten-no[1], [1]*Graduate School of Information Science, Nagoya University, Japan*

PP270 **MP2-F12 Methods in Turbomole**
Sebastian Höfener[1], Florian A. Bischoff[1], Andreas Glöß[1], David P. Tew[1], Wim Klopper[1], [1]*Institut für Physikalische Chemie, Universität Karlsruhe, Germany*

PP271 **A Virtual Way to Explicit Inclusion of Anharmonicity in Thermal Averages and Thermochemical Properties**
Mikkel Bo Hansen[1], Ove Christiansen[1], Daniele Toffoli[1], Jacob Kongsted[2], [1]*The Lundbeck Foundation Center for Theoretical Chemistry and Center for Oxygen Microscopy and Imaging, Department of Chemistry, University of Aarhus, Denmark,* [2]*Department of Theoretical Chemistry, Chemical Center, University of Lund, Sweden*

PP272 **MD and QM/MM Studies of Far-Red Fluorescent Protein HcRed**
Qiao Sun[1], Markus Doerr[2], Sean Smith[1], Walter Thiel[2], [1]*Centre for Computational Molecular Science, Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, Australia,* [2]*Max-Planck-Institut fur Kohlenforschung, Germany*

PP273 **Combination of Molecular Docking and Quantum Chemical Calculations for Understanding the Binding Interaction of HIV-1 RT Inhibitors of Diarylpyrimidine Derivatives in the WT and K103N HIV-1 RT Binding Pockets**
Pornpan Pungpo[1], Auradee Punkvang[1], Patchreenart Saparpakorn[2], Supa Hannongbua[2], [1]*Faculty of Science, Ubonratchathani University, Thailand,* [2]*Faculty of Science, Kasetsart University, Thailand*

PP274 **Structure and Conformational Analysis of some Oligomers of 2-Br and 4-Br Styrenes. An Approach to the Quantum Description of Polymer Macroscopic Properties**
Manuel Fernández-Gómez[1], Maria Paz Fernández-Liencres[1], Amparo Navarro[1], Tomás Peña[1], José Manuel Granadino[1], Andrés Garzón[1], María J. Sanchis[2], Gustavo Domínguez-Espinosa[2], [1]*University of Jaén, Department of Physical and Analytical Chemistry, Spain,* [2]*Polytechnics University of Valencia, Department of Applied Thermodynamics, Spain*

PP275 **Nature of the Vinyl and the Methyl Torsional Barriers in 2, 3 and 4-Methyl Styrenes. An Approach to the Structural Analysis**
Manuel Fernández-Gómez[1], Manuel Quesada Rincón[1], José Manuel Granadino-Roldán[1], Amparo Navarro[1], Tomás Peña Ruiz[1], Andrés Garzón[1], Maria Paz Fernández-Liencres[1], [1]*University of Jaén, Department of Physical and Analytical Chemistry, Spain*

PP276 **Investigation of the I21V and S94A Mutation Influence on INH–NAD and NADH Binding to InhA Enzyme, Based on Quantum Chemical Calculations**
Auradee Punkvang[1], Patchreenart Saparpakorn[2], Supa Hannongbua[2], Pornpan Pungpo[1], [1]*Faculty of Science, Ubonratchathani University, Thailand,* [2]*Faculty of Science, Kasetsart University, Thailand*

PP277 **Asymmetric Hydrogenation with Rh^+ Catalysts. A DFT Study on the Influence of Freely-Rotating bis-Phenyl Substituents on Enantioselectivity**
Feliu Maseras[1], Steven Donald[1], [1]*Institute of Chemical Research of Catalonia (ICIQ), Spain*

PP278 **A Molecular Approach to Ligand-Receptor Interaction: Insights from Molecular Dynamics Simulations**
Francesca Collu[1], Matteo Ceccarelli[1], Paolo Ruggerone[1], [1]*CNR-INFM SLACS, Cosmolab, and Physics Department, University of Cagliari, Italy*

PP279 **Affordable Modelling of H-Bonded Solutes using MD-ONIOM2**
Veeramol Vailikhit[1], Wilhelm Josef Holzschuh[1], Supa Hannongbua[2], [1]*Faculty of Liberal Arts and Science, Kasetsart University, Kamphaeng Saen Campus, Thailand,* [2]*Department of Chemistry, Faculty of Science, Kasetsart University, Thailand*

PP280 **DMRG Calculations on Relative Energies of Transition Metal Clusters**
Konrad Heinrich Marti[1], Gerrit Moritz[1], Markus Reiher[1], [1]*Laboratory of Physical Chemistry, ETH Zürich, Switzerland*

PP281 **Catecholase Activity: Model Complexes and Mechanistic Insights**
Amsaveni Muruganantham[1], Peter Comba[1], [1]*Inorganic Chemistry, Germany*

PP282 **Pyrite Chemistry from First Principles Simulations**
András Stirling[1], [1]*Chemical Research Center, Hungary*

PP283 **Enhancing Anion-π Interactions between Neutral Molecular Tweezers and Anions**
Jose M. Hermida-Ramón[1], Marcos Mandado-Alonso[1], Marta Sánchez-Lozano[1], Carlos M. Estévez[1], [1]*Depto. Química Física. University of Vigo., Spain*

PP284 **QM/MM Study of the Sulfoxidation Reaction of Cytochrome $P450_{BM3}$**
Cristina S. Porro[1], Michael J. Sutcliffe[1], Samuel P. de Visser[1], [1]*Manchester University, Manchester Interdisciplinary Biocentre, United Kingdom*

PP285 **Computing Protein NMR Properties without Empirical Hypersurfaces – A Novel Approach Based on Bond Polarization Theory**
Igor Jakovkin[1], Ulrich Sternberg[1], Anne S. Ulrich[1], [1]*Karlsruhe Institute of Technology, IBG, Germany*

PP286 **Enzyme Inhibitor Trend Analysis (EITA)**
Michael Shokhen[1], Netaly Khazanov[1], Amnon Albeck[1], [1]*Bar Ilan University & Department of Chemistry, Israel*

Poster Session 2 – Monday September 15 – 5.30-7.30pm

PP287 **Extrapolating Potential Energy Surfaces by Scaling Electron Correlation: Isomerization of Bicyclobutane to Butadiene**
Jesse Lutz[1], Piotr Piecuch[1], [1]*Department of Chemistry, Michigan State University, United States*

PP288 **Anharmonic Vibrational Calculations for Small Molecules and Polymers**
Murat Keceli[1], Kiyoshi Yagi[2], So Hirata[1], [1]*University of Florida Quantum Theory Project, Department of Physics and Department of Chemistry, United States,* [2]*University of Tokyo Department of Applied Chemistry, Graduate School of Engineering, Japan*

PP289 **Identification of Superheavy Elements by γ-Spectroscopy**
Christian Thierfelder[1], Peter Schwerdtfeger[1], [1]*Centre of Theoretical Chemistry and Physics, New Zealand Institute for Advanced Study, Massey University, New Zeala*

PP290 **Relativistic Effects in Homogeneous Catalysis with Au(III) – Addition of Water to Propyne**
Matthias Lein[1], Peter Schwerdtfeger[1], [1]*Centre of Theoretical Chemistry and Physics, New Zealand Institute for Advanced Study, Massey University, New Zealand*

PP291 **Linear Agostic Interactions – Is Side-On Coordination Necessary?**
Matthias Lein[1], Alastair J. Nielson[2], John A. Harrison[2], [1]*Centre of Theoretical Chemistry and Physics, New Zealand Institute for Advanced Study, Massey University, New Zealand,* [2]*Department of Chemistry, Institute of Fundamental Sciences, Massey University, New Zealand*

PP292 **Quantum Dynamical Simulations of Intense Laser Field Interactions with Atoms and Small Molecules: A High-Harmonic Generation as an Example**
Olena Ponomarenko[1], [1]*The University of Melbourne, The School of Physics, ARC CoE CXS, Australia*

PP293 **Knowledge-Based Approaches to Protein Assembly**
Hong Ching Lee[1], Hong Wing Lee[1], William Bret Church[1], [1]*University of Sydney, Faculty of Pharmacy, Australia*

PP294 **In-Situ Spectroscopic Study for Fine Chemical Syntheses: Combination of Spectral Reconstruction and DFT Calculation**
Feng Gao[1], Shuying Cheng[1], Marc Garland[1], [1]*Process Science & Modelling, Institute of Chemical and Engineering Sciences, Singapore*

PP295 **Locating Minimum Energy Crossing Points Using EOM–CC Methods**
Evgeny Epifanovsky[1], Anna Krylov[1], [1]*Department of Chemistry, University of Southern California, United States*

PP296 **The Relationship between Spectroscopic Transition Energies and the Redox Potentials of Chlorophylls a, b, d and Bacterio-Chlorophyll a**
Zheng-Li Cai[1], Jeffrey R. Reimers[1], Min Chen[2], [1]*School of Chemistry, The University of Sydney, Australia,* [2]*School of Biological Sciences, The University of Sydney, Australia*

PP297 **High Throughput Free Energy Calculations: Application to Solvation Free Energy Estimation**
Alpeshkumar Malde[1], Alan Mark[1], Alan Mark[2], [1]*School of Molecular and Microbial Science, Australia,* [2]*Institute of Molecular Bioscience, Australia*

PP298 **Optimising Numerical Atomic Orbital Basis Sets for the First Principles Modelling of Metal-Organic Frameworks**
Evelyne Deplazes[1], Julian Gale[2], [1]*University of Western Australia, School of Biomedical, Biomolecular and Chemical Sciences, Australia,* [2]*Curtin University of Technology, Nanochemistry Research Institute, Australia*

PP299 **The Mechanistic Study of Thermal Decomposition Mechanisms of Methylamine, Ethylamine and 1-Propylamine on Si(100) Surface**
Ji Eun Cho[1], Cheol Ho Choi[1], [1]*Department of Chemistry, College of Natural Sciences, Kyungpook National University, Korea, Republic of*

PP300 **The Significant Effect of External Water in Tautomerization Reactions – A Comparative Ab Initio Study of 2-Hydroxypyridine-$(H_2O)_n$ (n=0-3) and o-Hydroxyaryl Ketimine-$(H_2O)_n$ (n=0-2) in their Ground State**
Mohammad Harun Or Rashid[1], Cheol Ho Choi[1], [1]*Department of Chemistry, College of Natural Sciences, Kyungpook National University, Korea, Republic of*

PP301 **Supramolecular Porphyrin-Fullerene Interactions**
Peter Boyd[1], [1]*Chemistry Department, The University of Auckland, New Zealand*

PP302 **Solvation Effects for Polarizable Force Fields: Introducing Generalized Born Formula into the New Charge Equilibration Approach**
Naofumi Nakayama[1], Kazuo Ohta[1], Hitoshi Goto[2], [1]*Conflex Corporation, Japan,* [2]*Toyohashi University of Technology, Japan*

PP303 **The CC2-GHO Method for QM/MM Excited State Calculation**
Yukio Kawashima[1], Jaewoon Jung[2], Seiichiro Ten-no[2], [1]*Organization for the Promotion of Advanced Research, Kyushu University, Japan,* [2]*Graduate School of Information Science, Nagoya University, Japan*

PP304 **Comparative Study of Physisorption and Chemisorption of Hydrogen Molecules on Organometallic Compounds using Density Functional Theory**
Min Hee Park[1], Yoon Sup Lee[1], [1]*KAIST, Korea, Republic of*

PP305 **The Adsorption and Oxidation of NH_x (x = 1-3) on the RuO_2(110) Surface**
Jyh-Chang Jiang[1], Chia-Ching Wang[1], Ya-Jen Yang[1], [1]*National Taiwan University of Science and Technology, Department of Chemical Engineering, Taiwan*

PP306 **Mapping the Common Origins of Ion Selectivity in Biological Molecules**
Michael Thomas[1], Dylan Jayatilaka[1], Ben Corry[1], [1]*Biomedical, Biomolecular and Chemical Sciences, University of Western Australia, Australia*

PP307 **Towards Turning Australian Computational Chemists into eResearchers**
Sean Fleming[1], Florian Goessmann[1], Andrew Rohl[1], Vladislav Vassiliev[2], [1]*iVEC, 'The hub of advanced computing in Western Australia', Australia,* [2]*Australian National University Supercomputing Facility, Australia*

PP308 **Capturing Short- and Long-Range Correlation Effects using Intracule Functional Theory**
Deborah Crittenden[1], Peter Gill[1], [1]*Research School of Chemistry, Australian National University, Australia*

PP309 **The Nature of Proton Conduction in a Polymer Electrolyte Membrane, Nafion**
Yoong-Kee CHoe[1], Eiji Tsuchida[1], Tamio Ikeshoji[1], Shunsuke Yamakawa[2], Shi-aki Hyodo[2], [1]*AIST, Japan,* [2]*Toyota Central R&D Labs., Japan*

PP310 **Formation of Thiol-Gold Self-Assembled Monolayers**
Yun Wang[1], Noel Hush[2], Jeffrey Reimers[1], [1]*School of Chemistry, Australia,* [2]*School of Molecular and Microbial Biosciences, Australia*

PP311 **The Interaction of Hydrogen with Lithium-Doped Metal-Organic Framework 5**
Stephen Kolmann[1], Bun Chan[1], Meredith Jordan[1], [1]*School of Chemistry, The University of Sydney, Australia*

PP312 **Roaming Dynamics in Acetaldehyde Photodissociation**
Brianna Heazlewood[1], Meredith Jordan[1], Scott Kable[1], [1]*School of Chemistry, The University of Sydney, Australia*

PP313 **The Radiative Potential Method and Calculations of Radiative Corrections to Heavy Atom Properties**
Victor Flambaum[1], Jacinda Ginges[1], [1]*School of Physics, University of New South Wales, Australia*

PP314 **Projector Monte Carlo Method Based on Configuration State Functions**
Yuhki Ohtsuka[1], Shigeru Nagase[1], [1]*Department of Theoretical and Computational Molecular Science, Institute for Molecular Science, Japan*

PP315 **Coenzyme B_{12}-Dependent Fermentation of Glycerol – A Computational Study**
Danijela Baric[1], Gregory M. Sandala[2], Leo Radom[2], David M. Smith[1], [1]*Rudjer Boškovic Institute, Department for Organic Chemistry and Biochemistry, Croatia,* [2]*School of Chemistry, University of Sydney, Australia*

PP316 **A First Principles Study of Relativistic Effects in Bulk Group 12 Oxides**
Susan Biering[1], Peter Schwerdtfeger[1], [1]*Centre of Theoretical Chemistry and Physics, Massey University, New Zealand*

Poster Session 2 – Monday September 15 – 5.30-7.30pm

PP317 **The Reaction of a Grignard Reagent with Acetone in Solution: A Theoretical Study**
Toshifumi Mori[1], Shigeki Kato[1], [1]*Department of Chemistry, Graduate School of Science, Kyoto University, Japan*

PP318 **Melting of Small Aluminium Clusters**
Akin Budi[1], David J. Henry[1], Julian D. Gale[2], Irene Yarovsky[1], [1]*Applied Physics, School of Applied Sciences, RMIT University, Australia,* [2]*Nanochemistry Research Institute, Curtin University of Technology, Australia*

PP319 **Photo-Isomerization of XYO (X, Y = Cl, Br) using CCSD/EOM-CCSD Method**
KunHye Lee[1], Heesun An[1], Kyoungkoo Baeck[1], [1]*Department of Chemistry, Kangnung National University, Korea, Republic of*

PP320 **First Principle Calculations of Very Large Nanostructures**
Burak Cankurtaran[1], Julian Gale[1], Mike Ford[2], [1]*Nanochemistry Research Institute, Curtin University of Technology, Australia,* [2]*Institute for Nanoscale Technology, University of Technology, Sydney, Australia*

PP321 **Haemoglobin Revisited**
Don Vanselow[1], [1]*nativeproteins.blogspot.com, Australia*

PP322 **Fragment Molecular Orbital Method-Based Molecular Dynamics (FMO-MD) as a Simulator for Chemical Reactions in Explicit Solvation**
Yuto Komeiji[1], Makoto Sato[2], Takeshi Ishikawa[2], Yuji Mochizuki[2], Hiroshi Yamataka[2], Tatsuya Nakano[3], [1]*AIST, Japan,* [2]*Rikkyo Univ., Japan,* [3]*NIHS, Japan*

PP323 **Structural Modelling, Docking, and QM/MM Study of Ligand-binding upon Human AhR**
Sundaram Arulmozhiraja[1], Yohsuke Hagiwara[2], Masaru Tateno[2], Takahisa Ohno[3], [1]*National Institute for Materials Science, International Center for Materials Nanoarchitectonics, Japan,* [2]*University of Tsukuba, Center for Computational Sciences, Division of Materials and Life Sciences, Japan,* [3]*National Institute for Materials Science, Computational Materials Science Center & International Center for Materials Nanoarchitectonics, Japan*

PP324 **A PBC-DFT Study of π-Conjugation Polymer-Based Materials**
Bo-Cheng Wang[1], Wen-Hao Chen[1], [1]*Chemistry Department, Tamkang University, Taiwan*

PP325 **A New Approach for Multiconfigurational Density Functional Theory**
Takao Tsuneda[1], [1]*Department of Applied Chemistry, Graduate School of Engineering, University of Tokyo, Japan*

PP326 **Ligand-to-Metal Charge Transfer Dynamics in Blue Copper Protein Plastocyanin: A Molecular Dynamics Study**
Koji Ando[1], [1]*Department of Chemistry, Graduate School of Science, Kyoto University, Japan*

PP327 **Interaction Analysis between the EGF Receptor and EGF by FMO Calculation**
Toshio Watanabe[1], Takayoshi Ishimoto[1], Yutaka Tamura[3], Yuichi Inadomi[4], Hiroaki Umeda[1], Umpei Nagashima[1], [1]*Research Institute for Computational Science, National Institute of Advanced Industrial Science and Technology, Japan,* [2]*Japan Science and Technology Agency, Japan,* [3]*Department of Bioinformatics, Graduate School of Medicine, Chiba University, Japan,* [4]*Institute of Systems, Information Technologies and Nanotechnologies, Japan*

PP328 **The Diffusion Pathways of Phosphorus Atoms in the Silicon (001) Surface**
Jennifer Bell[1], Oliver Warschkow[1], Nigel Marks[1], David McKenzie[1], [1]*Centre for Quantum Computer Technology, School of Physics, The University of Sydney, Australia*

PP329 **QSAR study of Flavonoids Active against HT-29 Colon Carcinoma**
Bo-Cheng Wang[1], Yeong-Sheng Chang[1], [1]*Chemistry Department, Tamkang University, Taiwan*

PP330 **The 1^1B_u Lifetime of Short All-Trans Polyenes: A Theoretical Study**
Wilfredo Credo Chung[1], Shinkoh Nanbu[2], Toshimasa Ishida[1], [1]*Fukui Institute for Fundamental Chemistry, Kyoto University, Japan,* [2]*Computing and Communications Center, Kyushu University, Japan*

PP331 **DFT Study on Charge Conductivity of the DNA Duplex and Au Electrodes System**
Takayuki Tsukamoto[1], Yasuyuki Ishikawa[2], Hajime Wakabayashi[1], Yasuo Sengoku[1], Noriyuki Kurita[1], [1]*Department of Knowledge-Based Information Engineering, Toyohashi University of Technology, Japan,* [2]*Department of Chemistry, University of Puerto Rico, United States*

PP332 **Simultaneous Analytical Optimization of Variational Parameters in GTFs with the Full-CI of MC_MO Method: Application to Isotopomers of the Hydrogen Molecule**
Takayoshi Ishimoto[1], Masanori Tachikawa[2], Hiroaki Umeda[1], Toshio Watanabe[1], Umpei Nagashima[1], *[1]Research Institute for Computational Science, National Institute of Advanced Industrial Science and Technology, Japan, [2]Quantum Chemistry Division, Graduate School of Science, Yokohama-City University, Japan*

PP333 **Basis Set and Correlation Effects on Intracules**
Jason Pearson[1], Deborah Crittenden[1], Peter Gill[1], *[1]Research School of Chemistry, Australian National University, Australia*

PP334 **Self-Consistent Field Excited States**
Andrew Gilbert[1], Nicholas Besley[2], Peter Gill[1], *[1]Research School of Chemistry, The Australian National University, Australia, [2]School of Chemistry, The University of Nottingham, United Kingdom*

PP335 **Systematic Exploration on the Potential Energy Surface of Silicon Hydride and Germanium Hydride by the Anharmonic Downward Distortion Following Method**
Masahiro Moteki[1], Satoshi Maeda[1], Koichi Ohno[1], *[1]Department of Chemistry, Tohoku University, Japan*

PP336 **Alternative Algorithm of the Local Electron Correlation Method with the Region-Dividing Approach**
Wataru Mizukami[1], Yuki Kurashige[1], Takeshi Yanai[1], *[1]Department of Theoretical and Computational Molecular Science, Institute for Molecular Science, Japan*

PP337 **Solid State DFT Investigation of Porous Formate Magnetic Sponges, $[M_3(HCO_2)_6]$ and $[M_3(HCO_2)_6]:X$**
Sharon A. Rivera[1], Gordon Kearley[2], John A. Stride[1], *[1]University of New South Wales, School of Chemistry, Australia, [2]Bragg Institute, ANSTO, Australia*

PP338 **Grid-Enabled Large Fock Matrix Construction for FMO-MO Calculation**
Hiroaki Umeda[1], Toshio Watanabe[1], Yuichi Inadomi[3], Takayoshi Ishimoto[1], Umpei Nagashima[1], *[1]RICS, National Institute of Advanced Industrial Science and Technology (AIST), Japan, [2]CREST, Japan Science and Technology Agency (JST), Japan, [3]Institute of Systems, Information Technologies and Nanotechnologies, Japan*

PP339 **Jamberoo: Flexible Environment for Computational Chemistry**
Vladislav Vassiliev[1], *[1]The Australian National University, Supercomputer Facility, Australia*

PP340 **Structure and Bonding of the MCN Molecules, M=Cu, Ag, Au, Rg**
Patryk Zaleski-Ejgierd[1], Michael Patzschke[1], Pekka Pyykkö[1], *[1]University of Helsinki, Department of Chemistry, Finland*

PP341 **Efficient Construction of Global Potential Functions by a New Polynomial Fitting Technique and the Anharmonic Downward Distortion Following Method**
Yuto Osada[1], Satoshi Maeda[1], Koichi Ohno[1], *[1]Tohoku University, Japan*

PP342 **Probing the Structure and Dynamics of RNA Dinucleoside Monophosphates (ApA, ApC, CpA, CpC) with NMR Spectroscopy**
Zuzana Vokacova[1], Bohdan Schneider[2], Milos Budesinsky[2], Ivan Rosenberg[2], Vladimir Sychrovsky[2], Jiri Sponer[3], *[1]Charles University in Prague, Faculty of Mathematics and Physics, Czech Republic, [2]Institute of Organic Chemistry and Biochemistry AS CR, v.v.i., Czech Republic, [3]Institute of Biophysics AS CR, v.v.i., Czech Republic*

PP343 **Theoretical Study of Electron and Hydrogen Attachment to Disulphide Derivatives**
Jose A. Gamez[1], Luis Serrano-Andrés[2], Otilia Mo[1], Manuel Yáñez[1], *[1]Departamento de Quimica. Universidad Autonoma de Madrid. Cantobalnco 28049, Spain, [2]Universidad de Valencia. Instituto de Ciencia Molecular 22085, ES-46071, Spain*

PP344 **Comparative Theoretical Study of Hexagonally Crystallizing Metals and Laves Phases**
Dirk Andrae[1], Elena Voloshina[1], Beate Paulus[1], Nicola Gaston[2], Ulrich Wedig[3], Martin Jansen[3], *[1]Physical and Theoretical Chemistry, Freie Universität Berlin, Germany, [2]Industrial Research Ltd., Gracefield Research Center, New Zealand, [3]Max Planck Institute for Solid State Research, Germany*

PP345 **The Stationary States of the Two-Electron Atoms**
Dirk Andrae[1], *[1]Physical and Theoretical Chemistry, Freie Universität Berlin, Germany*

Poster Session 2 – Monday September 15 – 5.30-7.30pm

PP346 **A Grid System for the Structure-Activity Relationship Study**
Undram Damdinsuren[1], Shin-ya Takane[1], *[1]Department of Information Systems Engineering, Osaka Sangyo University, Japan*

PP347 **On the Intermolecular Energy Transfer around Vibrationally Excited Hydrogen Fluoride in Aqueous Solution: A Molecular Dynamics Simulation Study**
Takuya Okamoto[1], Masataka Nagaoka[1], *[1]Graduate School of Information Science, Nagoya University, Japan*

PP348 **De Novo Design and Virtual Screening of Nonlinear Materials for All-Optical Signal Processing**
Alexander Oliferenko[1], Vladimir Palyilin[1], Nikolay Zefirov[1], Artem Masunov[2], *[1]Department of Chemistry, Moscow State University, Russian Federation, [2]Nanoscience Technology Center, Department of Chemistry and Department of Physics, University of Central Florida, United States*

PP349 **Polarizable Force Field YFF2: Towards Multi-Scale Simulations of Nano-Sized Objects**
Alexander Oliferenko[1], Dmitri Shulga[1], Serge Pisarev[1], Vladimir Palyulin[1], Nikolay Zefirov[1], Alexander Yakovenko[2], Vladimir Bdzhola[2], *[1]Department of Chemistry, Moscow State University, Russian Federation, [2]Institute of Molecular Biology and Genetics of National Academy of Sciences of Ukraine, Ukraine*

PP350 **Local Correlation Calculations using Cluster-In-Molecule Standard and Renormalized Coupled-Cluster Methods**
Wei Li[1], Piotr Piecuch[1], Jeffrey R. Gour[1], *[1]Department of Chemistry, Michigan State University, United States*

POSTER SESSION 3 – TUESDAY SEPTEMBER 15 – 5.30-7.30pm

PP351 **Regioselectivity in the Heck Reaction**
Carina Bäcktorp[1], Signe Teuber Henriksen[1], Per-Ola Norrby[1], [1]*University of Gothenburg, Department of Organic Chemistry, Sweden,* [2]*Technical University of Denmark, Denmark*

PP352 **Air Oxidation of Ethoxylated Surfactants – Computational Estimations of Energies and Reaction Behaviors**
Carina Bäcktorp[1], Anna Börje[1], J. Lars G. Nilsson[1], Ann-Therese Karlberg[1], Per-Ola Norrby[1], Gunnar Nyman[1], [1]*Department of Chemistry, University of Gothenburg, Sweden,* [2]*Göteborg Science Centre for Molecular Skin Research, Faculty of Science, University of Gothenburg, Sweden*

PP353 **The Amino Group in Adenine. Is it Co-planar with the Molecular Rings or Not?**
Wiktor Zierkiewicz[1], Danuta Michalska[1], Ludwik Komorowski[1], Jiří Černý[2], Pavel Hobza[2], [1]*Wroclaw University of Technology, Faculty of Chemistry, Poland,* [2]*Academy of Sciences of the Czech Republic, Institute of Organic Chemistry and Biochemistry, Czech Republic*

PP354 **ChemIME: An Input Method Engine for Chemists**
Haruka Tkeuchi[1], Xu Yang[1], Shin-ya Takane[1], [1]*Department of Information Systmes Engineering, Osaka Sangyo University, Japan*

PP355 **Ab Initio Calculations of the Zero-Field Splitting Tensors of Organic Open-Shell Molecules**
Kenji Sugisaki[1], Kazuo Toyota[1], Kazunobu Sato[1], Daisuke Shiomi[1], Takeji Takui[1], [1]*Departments of Chemistry and Materials Science, Graduate School of Science, Osaka City University, Japan*

PP356 **A Chemically Reasonable Model of Various Phosphine Ligands: Application of CCSD(T) Calculation to Large Transition Metal Complexes**
Yu-Ya Ohnishi[1], Mayu Nakaoka[1], Yoshihide Nakao[1], Hirofumi Sato[1], Shigeyoshi Sakaki[1], [1]*Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, Japan*

PP357 **A DFT Study on a Natural Diels-Alder Reaction**
Sadra Kashefolgheta[1], Mehdi Irani[1], Mohammad Reza Gholami[1], [1]*Department of Chemistry-Sharif University of Technology, Iran, Islamic Republic of*

PP358 **Structure and Vibrational Spectra of Hydrogen-Bonded Clusters by the Anharmonic Downward Distortion Following Method**
Satoshi Maeda[1], Yu Watanabe[1], Yi Luo[1], Koichi Ohno[1], [1]*Department of Chemistry, Graduate School of Science, Tohoku University, Japan*

PP359 **Analysis of an Electronic Spectrum using the Ab Initio Path Integral Molecular Dynamics Method**
Masataka Sugimoto[1], Motoyuki Shiga[2], Masanori Tachikawa[1], [1]*Graduate School of Integrated Science, Yokohama City University, Japan,* [2]*Japan Atomic Energy Agency, Japan*

PP360 **Computational Study of the Sonogashira Cross-Coupling Reaction in the Gas Phase**
Peeter Burk[1], Jaana Tammiku-Taul[1], Lauri Sikk[1], Andras Kotschy[2], [1]*Institute of Chemistry, University of Tartu, Estonia,* [2]*Institute of Chemistry, Eötvös Loránd University, Hungary*

PP361 **Identification of an Aryloxenium Ion by Time Resolved Resonance (TR^3) Spectroscopy and Density Functional Theory: First Vibrational Spectrum of an Oxenium Ion**
Stephen Glover[1], Michael Novak[2], Yue-Ting Wang[2], David Phillips[3], Jiadan Xue[3], [1]*University of New England, School of Science and Technology, Australia,* [2]*Miami University, Department of Chemistry and Biochemistry, United States,* [3]*Hong Kong University, Department of Chemistry, China*

PP362 **Molecular Dynamic Simulations Can Complement Experiments to Probe Antibiotics Diffusion through Bacterial Porins**
Eric Hajjar[1], Amit Kumar[1], Enrico Spiga[1], Francesca Collu[1], Paolo Ruggerone[1], Matteo Ceccarelli[1], [1]*Department of Physics, University of Cagliari., Italy*

PP363 **Avoiding Heisenberg with Certainty**
Yves A. Bernard[1], Peter M. W. Gill[1], [1]*Research School of Chemistry, Australian National University, Australia*

PP364 **Parallel Implementation of RI-MP2 Energy Calculations of Large Molecules**
Michio Katouda[1], Shigeru Nagase[1], [1]*Department of Theoretical and Computational Molecular Science, Institute for Molecular Science, Japan*

Poster Session 2 – Tuesday September 16 – 5.30-7.30pm

PP365 **Development of an Efficient Computational Scheme for Relativistic GMC-QDPT and its Application to Molecular Systems**
Ryo Ebisuzaki[1], Yoshihiro Watanabe[1], Haruyuki Nakano[1], [1]*Department of Molecular Chemistry, Graduate School of Sciences, Kyushu University, Japan*

PP366 **Ab Initio Benchmark Calculations on Monoligand Ca(II) Complexes and Comparison with Density Functional Theory Methodologies**
Víctor M Rayón[1], Haydee Valdés[2], Natalia Díaz[2], Dimas Suárez[2], [1]*University of Valladolid, Department of Physical Chemistry and Inorganic Chemistry, Spain,* [2]*University of Oviedo, Department of Physical Chemistry and Analytical Chemistry, Spain*

PP367 **Aldehyde Dehydrogenase Enzymatic Chemistry: Insights from Hybrid QM/MM Calculations**
Troy Wymore[1], James Keener[1], Shawn Brown[1], [1]*Pittsburgh Supercomputing Center, National Resource for Biomedical Supercomputing, United States*

PP368 **Simulation Studies of the Folding and Aggregation of Model Amyloid Peptides in Solution and at an Interface**
Volker Knecht[1], Madeleine Kittner[1], Reinhard Lipowsky[1], [1]*Max Planck Institute of Colloids and Interfaces, Theory & Bio-Systems Department, Germany*

PP369 **Electrophoretic Mobility Does Not always Reflect the Charge on a Particle**
Volker Knecht[1], H. Jelger Risselada[1], Alan E. Mark[3], Siewert-Jan Marrink[2], [1]*Max Planck Institute of Colloids and Interfaces, Theory & Bio-Systems, Germany,* [2]*Groningen Biomolecular Sciences and Biotechnology Institute, and Zernike Institute for Advanced Materials, University of Groningen, Netherlands,* [3]*School of Molecular and Microbial Sciences, University of Queensland, Australia,* [4]*Groningen Biomolecular Sciences and Biotechnology Institute, and Zernike Institute for Advanced Materials, University of Groningen, Netherlands*

PP370 **A Multilevel Sidechain Representation Library for Protein Structure Prediction and Docking**
Quentin Kaas[1], [1]*Institute for Molecular Bioscience, University of Queensland, Australia*

PP371 **In Quest of an Efficient and Accurate Modelling of the Photochemistry of Biological Photoreceptors: A QM/MM Approach**
Pedro B. Coto[1], Israel González-Ramírez[1], Gloria Olaso-González[1], Daniel Roca-Sanjuán[1], Juan José Serrano-Pérez[1], Manuela Merchán[1], [1]*Instituto de Ciencia Molecular (ICMOL), University of Valencia, Spain*

PP372 **Efficient Extrapolation of Triple Excitations to the Complete Basis Set Limit**
Ericka Barnes[1], George Petersson[1], [1]*Wesleyan University, Chemistry Department, United States*

PP373 **Decomposition of 6,7,8-trioxybicyclo[3.2.2]nonane Prompted by Fe(II). A Model to Study the Fisrt Stages of the Decomposition Mechanism of Artemisinin**
Pamela Moles[1], V. Sixte Safont[1], Mónica Oliva[1], [1]*Universitat Jaume I, Departament de Química Física i Analítica, Spain*

PP374 **Solvation of Platinum Chloro-Complexes in 1,3-Dialkylimidazolium Ionic Liquids**
Gerhard A Venter[1], Kevin J Naidoo[1], [1]*Department of Chemistry, University of Cape Town, South Africa*

PP375 **Mechanistic Analysis of Intermolecular Arene C-H Activation**
Stuart A. Macgregor[1], David L. Davies[1], Amalia I. Poblador-Bahamonde[1], [1]*Heriot-Watt University, Engineering and Physical Sciences (EPS), United Kingdom*

PP376 **DFT Study on Charge Conductivity of DNA-Wrapped Carbon Nanotubes**
Noriyuki Kurita[1], Ikuyo Komura[1], Takayuki Tsukamoto[1], Yasuyuki Ishikawa[2], [1]*Toyohashi University of Technology, Japan,* [2]*University of Puerto Rico, United States*

PP377 **Specific Interactions between Thermolysin and Dipeptide Ligands Obtained by Fragment Molecular Orbital Calculations**
Noriyuki Kurita[1], Kenichi Dedachi[1], Mahmud T. H. Khan[2], Ingebrigt Sylte[2], [1]*Toyohashi University of Technology, Japan,* [2]*University of Tromsø, Norway*

PP378 **Characterization of Weak Interactions between Aromatic Amino Acids and the Natural Nucleobases**
Lesley Rutledge[1], Holly Durst[1], Stacey Wetmore[1], [1]*University of Lethbridge, Department of Chemistry and Biochemistry, Canada*

PP379 **DFT Study of the Manganese Containing Ribonucleotide Reductase in Chlamydia trachomatis**
Katarina Roos[1], Per E.M. Siegbahn[1], [1]*Department of Physics, Stockholm University, Sweden*

PP380 **Computational Studies of the Isomerisation of Nido- and Closo- 12-vertex Carboranes**
Stuart A. Macgregor[1], David McKay[1], Alan J. Welch[1], [1]*Heriot-Watt University, School of Engineering and Physical Sciences, United Kingdom*

PP381 **Short Intramolecular Hydrogen Bonds: Derivatives of Malonaldehyde with Symmetrical Substituents**
Jacqueline Hargis[1], Francesco Evangelista[1], Justin Ingels[1], Henry Schaefer[1], [1]*Center of Computational Chemistry, University of Georgia, United States*

PP382 **Structural Effects of DNA Modification at the C8 site of Purine Nucleobases**
Andrea Millen[1], Cassandra Churchill[1], Lex Navarro-Whyte[1], Jenny Shim[1], Katie Schlitt[2], Chris McLaughlin[2], Richard Manderville[2], Stacey Wetmore[1], [1]*Department of Chemistry & Biochemistry, University of Lethbridge, Canada,* [2]*Departments of Chemistry & Toxicology, University of Guelph, Canada*

PP383 **Chlorine-π interactions: New Methods for Old Problems**
Anna K. Croft[1], Helen M. Howard-Jones[1], Chris C. Wood[1], [1]*School of Chemistry, University of Wales Bangor, United Kingdom*

PP384 **The Importance of Solvent Reorganisation in Reactions Performed in Ionic Liquids**
Hon Man Yau[2], Susan A. Barnes[1], James M. Hook[2], Tristan G. A. Youngs[3], Jason B. Harper[2], Anna K. Croft[1], [1]*School of Chemistry, University of Wales Bangor, United Kingdom,* [2]*School of Chemistry, University of New South Wales, Australia,* [3]*Atomistic Simulation Centre, Queen's University Belfast, United Kingdom*

PP385 **Quantum Chemical Study on the Promotion Effect of H_2 in the Selective Catalytic Reduction of NOx over Ag-MFI Zeolite**
Kyoichi Sawabe[1], Ken-ichi Shimizu[1], Atsushi Satsuma[1], [1]*Department of Molecular Design and Engineering, Nagoya University, Japan*

PP386 **Towards a 32-electron Principle: Pu@Pb_{12} and Related Systems**
Jean-Pierre Dognon[1], Carine Clavaguéra[1], Pekka Pyykkö[1], [1]*CEA/Saclay, DSM/IRAMIS/SCM, France,* [2]*CNRS/Ecole Polytechnique, France,* [3]*University of Helsinki, Finland*

PP387 **Spin-Orbit Effects on Structures and Vibrational Frequencies of Haloiodomethane Cations and Halogentriflorides**
Hyoseok Kim[1], Yoon Sup Lee[1], [1]*KAIST, Korea, Republic of*

PP388 **Interference Partitioning of the Energy for Generalized Product Functions: N_2 as a Test Case**
Thiago Messias Cardozo[1], Marco Antonio Chaer Nascimento[1], [1]*Instituto de Química - UFRJ, Brazil*

PP389 **Canonical Transformation Theory: Review and Application to Transition Metal Oxides**
Eric Neuscamman[1], Takeshi Yanai[1], Garnet Chan[1], [1]*Cornell Department of Chemistry and Chemical Biology, United States,* [2]*Institute for Molecular Science, Japan,* [3]*Cornell Department of Chemistry and Chemical Biology, United States*

PP390 **Temperature and Isotope Effects on Water Cluster Ions with Path Integral Molecular Dynamics**
Suzuki Kimichi[1], Motoyuki Shiga[2], Tachikawa Masanori[1], [1]*Quantum Chemistry Division, Graduate School of Science, Yokohama-City University, Japan,* [2]*CCSE, Japan Atomic Energy Agency, Japan*

PP391 **Molecular Dynamics Simulation of Photodesorption Process of CO Ice**
Junko Takahashi[1], Marc van Hemert[2], [1]*Meiji Gakuin University, Japan,* [2]*Leiden Institute of Chemistry, University of Leiden, Netherlands*

PP392 **HERON Reaction of N-Acyloxy-N-alkoxyamides – Theoretical and Experimental Study**
Stephen Glover[1], [1]*School of Science and Technology, University of New England, Australia*

PP393 **A Linear-Scaling Spectral-Element Method for Computing Electrostatic Potentials**
Mark A. Watson[1], Kimihiko Hirao[1], [1]*Department of Applied Chemistry, The University of Tokyo, Japan*

PP394 **Automatized Derivation and String-Based Evaluation of Explicitly Correlated Wavefunctions**
Andreas Köhn[1], Gareth Richings[1], [1]*University of Mainz, Institute of Physical Chemistry, Germany*

PP395 **Conical for Stepwise, Glancing for Concerted: The Role of Excited State Topology in Three-body Dissociation of Sym-Triazine**
Vadim Mozhayskiy[1], Anna I. Krylov[1], [1]*University of Southern California, Chemistry Department, United States*

Poster Session 2 – Tuesday September 16 – 5.30-7.30pm

PP396 **Enzymic H-tunnelling – A Role for Promoting Vibrations?**
Linus O. Johannissen[1], Micheal J. Sutcliffe[1], Nigel S. Scrutton[2], [1]*School of Chemical Engineering and Analytical Science, Manchester Interdisciplinary Biocentre, University of Manchester, United Kingdom,* [2]*Faculty of Life Sciences, Manchester Interdisciplinary Biocentre, University of Manchester, United Kingdom*

PP397 **Calculation of the Effective Chemical Shielding Anisotropy in L-Alanyl-L-alanine, Conformational and Charge Dependence Study**
Ladislav Benda[1], Petr Bouř[1], Norbert Müller[2], Vladimír Sychrovský[1], [1]*Institute of Organic Chemistry and Biochemistry, Molecular Spectroscopy Group, Czech Republic,* [2]*Johannes Kepler University, Institute of Organic Chemistry, Austria*

PP398 **Insights into the Structural Basis of N2 and O6 Substituted Guanine Derivatives as Cyclin-Dependent Kinase 2 (CDK2) Inhibitors: Prediction of the Binding Modes and Potency by Docking and ONIOM Calculations**
Jans Alzate-Morales[1], Julio Caballero Ruiz[1], Ariela Vergara[1], Fernando Danilo González Nilo[1], [1]*Bioinformatics and Molecular Simulation Centre, University of Talca, Chile*

PP399 **New Implementation and Parallelization of DMRG: Towards Large-Scale Multireference Electronic-Structure Calculations**
Yuki Kurashige[1], Takeshi Yanai[1], [1]*Institute for Molecular Science, Japan*

PP400 **Hybrid Functionals and Møller-Plesset Perturbation Theory applied to Extended Systems**
Joachim Paier[1], Andreas Grueneis[1], Martijn Marsman[1], Georg Kresse[1], [1]*University of Vienna, Computational Materials Physics, Austria*

PP401 **Molecular Docking with Accurate Polarizable Charges: A QM/MM Approach in Discovery Studio**
Jiabo Li[1], Al Maynard[1], Jurgen Koska[1], George Fitzgerald[1], Dipesh Risal[1], Paul Kung[1], Jon Sutter[1], Paul Flook[1], [1]*Accelrys Inc, United States*

PP402 **Ionization Energy of the 1-Hydroxyethyl Radical: The Effects of Hyperconjugation**
Boris Karpichev[1], Hanna Reisler[1], Anna Krylov[1], Kadir Diri[1], [1]*University of Southern California, Department of Chemistry, United States*

PP403 **Oxidase Catalysis Beyond Biology: A Density Functional Theory Investigation of N-Methyl-Imidazole (and Acetate) Complexes of First-Row Transition Metal Ions**
Ivan Taylor[1], Stephen Colbran[1], Gary Willett[1], [1]*School of Chemistry, University of New South Wales, Australia*

PP404 **Development of the Translational and Rotational Free Quantum Monte Carlo Method**
Yukiumi Kita[1], Ryo Maezono[2], Masanori Tachikawa[1], [1]*Yokohama City University, Japan,* [2]*School of Information Science, Japan Advanced Institute of Science and Technology, Japan*

PP405 **Fragmentation of Peptide Radical Cations: Proton Scissors vs. Proton Patches**
Galina Orlova[1], Matthew MacLennan[1], [1]*St. Francis Xavier University, Department of Chemistry, Canada*

PP406 **A Molecular Dynamics Study of Protein-Protein Binding between a K^+ Channel and Peptide Toxin**
Po-Chia Chen[1], Serdar Kuyucak[1], [1]*School of Physics, The University of Sydney, Australia*

PP407 **A Molecule Search System Using Ajax**
Lizhu Liu[1], Shin-ya Takane[1], [1]*Department of Information Systems Engineering, Osaka Sangyo University, Japan*

PP408 **Ab Initio Calculation of the Coherent 2D Infrared Response Function for Two-Dimensional Vibrational Spectroscopy**
Sangjoon Hahn[1], Minhaeng Cho[2], [1]*Korea Science Academy, Korea, Republic of,* [2]*Korea University, Korea, Republic of*

PP409 **Ab Initio Density Matrix Renormalization Group with Orbital Optimisation and its Application to β-Carotene**
Debashree Ghosh[1], Johannes Hachmann[1], Takeshi Yanai[2], Garnet Chan[1], [1]*Department of Chemistry and Chemical Biology, Cornell University, United States,* [2]*Department of Theoretical and Computational Molecular Science, Institute for Molecular Science, Japan*

PP410 **Excited State Dynamics of Molecules using Gaussian Wave Packets**
Takashi Kuchitsu[1], Motoyuki Shiga[2], Masanori Tachikawa[1], [1]*International Graduate School of Arts and Sciences, Yokohama City University, Japan,* [2]*Center for Computational Science and E-Systems, Japan Atomic Energy Agency (JAEA), Japan*

PP411 **Spin Transition Mechanism and New Necessary Condition of LIESST: DFT Study of $[Fe(2\text{-}pic)_3]^{2+}$**
Hideo Ando[1], Yoshihide Nakao[1], Hirofumi Sato[1], Shigeyoshi Sakaki[1], [1]*Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, Japan*

PP412 **Molecular Dynamics Simulation for the Protonation Process in Matrix-Assisted Laser Desorption Ionization**
Makoto Hatakeyama[1], Masanori Tachikawa[1], [1]*Graduate School of Integrated Science, Yokohama-City University, Japan*

PP413 **Tungsten η^3-Silaallyl/Vinylsilyl, η^3-Silapropargyl/Alkynylsilyl, and Silylene Complexes: New Insight of their Bonding Nature and Electronic Structure**
Mausumi Ray[1], Yoshihide Nakao[1], Hirofumi Sato[1], Shigeyoshi Sakaki[1], [1]*Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, Japan*

PP414 **Theoretical Analysis of Positron Halide Complexes by Multi-Component Quantum Monte Carlo Method**
Tomohiro Takeda[1], Yukiumi Kita[1], Ryo Maezono[2], Masanori Tachikawa[1], [1]*Graduate School of Integrated Science, Yokohama City University, Japan,* [2]*School of Information Science, Japan Advanced Institute of Science and Technology, Japan*

PP415 **New Developments in Spin-Flip Methods**
David Casanova[1], Lyudmila V. Slipchenko[2], Anna I. Krylov[3], Martin Head-Gordon[1], [1]*University of California, Berkeley, United States,* [2]*Purdue University, United States,* [3]*University of Southern California, United States*

PP416 **Fullerene Formation from a Benzene Source: Density Functional Tight-Binding Molecular Dynamics Simulations**
Biswajit Saha[1], Stephan Irle[2], Keiji Morokuma[1], [1]*Fukui Institute for Fundamental Chemistry, Kyoto University, Japan,* [2]*Institute for Advanced Research and Department of Chemistry, Nagoya University, Japan*

PP417 **The Electronic Structure of Gold Clusters: A Study by Coupled Cluster Calculation with a Newly Developed Relativistic Model Core Potential**
Hirotoshi Mori[1], Hisaki Nakashima[2], Eisaku Miyoshi[2], [1]*Division of Advanced Sciences, Ochadai Academic Production, Ochanomizu University, Japan,* [2]*Interdisciplinary Graduate School of Engineering Sciences, Kyushu University, Japan*

PP418 **Density Functional Theory Study on the Stacking and Excitation of Metal Ion Containing Artificial DNA**
Hideaki Miyachi[1], Toru Matsui[1], Yasuteru Shigeta[2], Kimihiko Hirao[1], [1]*Department of Applied Chemitry, School of Engineering, The University of Tokyo, Japan,* [2]*Institute of Picobiology, Graduate School of Lifescience, University of Hyogo, Japan*

PP419 **Diels-Alder Reaction of Crotonyl Phosphonate: Cylopentadiene versus Cyclohexadiene**
Nihan Çelebi-Ölçüm[1], Viktorya Aviyente[1], K. N. Houk[2], [1]*Bogaziçi University, Department of Chemistry, Turkey,* [2]*University of California, Los Angeles Department of Chemistry and Biochemistry, United States*

PP420 **Solving the Schrödinger Equation of the Hydrogen Molecular Ion in a Magnetic Field by the Free ICI (Iterative Complement Interaction) Method**
Atsushi Ishikawa[1], Hiroyuki Nakashima[2], Hiroshi Nakatsuji[2], [1]*Kyoto University, Japan,* [2]*Quantum Chemistry Research Institute, JST-CREST, Japan*

PP421 **Oxygen Atom Transfer Reactions of Iridium and Osmium Complexes: Theoretical Study of Significantly Large Differences between these Two Complexes**
Atsushi Ishikawa[1], Yoshihide Nakao[1], Hirofumi Sato[1], Shigeyoshi Sakaki[1], [1]*Kyoto University, Japan*

PP422 **Elucidating the Photoelectron Spectrum of CS by Molecular Vibration Calculations of CS^+**
Nobumitsu Honjou[1], [1]*Oita University, Japan*

PP423 **DFT Studies into Conjugate Transfer Hydrogentations of Hantzsch Esters**
Robert S Paton[1], Jonathan M Goodman[1], [1]*University of Cambridge, United Kingdom*

Poster Session 2 – Tuesday September 16 – 5.30-7.30pm

PP424 **Theory of Paramagnetic NMR Chemical Shift in the Presence of ZeroField Splitting**
Teemu O. Pennanen[1], Juha Vaara[1], [1]*Laboratory of Physical Chemistry, Department of Chemistry, University of Helsinki, Finland*

PP425 **Reversible Interconversion of H_2 and H_2O by a Hydroxo/Sulfido-Bridged Dinuclear Ruthenium-Germanium Complex. Theoretical Study**
Noriaki Ochi[1], Hirofumi Sato[1], Yoshihide Nakao[1], Shigeyoshi Sakaki[1], [1]*Kyoto University, Department of Molecular Engineering, Japan*

PP426 **Theoretical Study of the Hydrogen Bonds in Functionalized Molecules using Multi-Component Molecular Orbital (mc_mo) Method**
Masato Kaneko[1], Taro Udagawa[2], Masanori Tachikawa[1], [1]*Graduate School of Integrated Science, Yokohama-City University, Japan,* [2]*Faculty of Engineering, Gifu University, Japan*

PP427 **Role of Electrodes in Characterizing the Transport Properties of a Molecular Device**
Yeonchoo Cho[1], Woo Youn Kim[1], Kwang Soo Kim[1], [1]*Center for Superfunctional Materials, Department of Chemistry, Pohang University of Science and Technology, Korea, Republic of*

PP428 **The CASPT2 Method: Current Limitations and Benchmarks**
Valera Veryazov[1], [1]*Lund University, Theoretical Chemistry, Sweden*

PP429 **Cycloaddition Reactions of ICNO: A Theoretical and Experimental Study**
Melinda Krebsz[1], Tibor Pasinszki[1], Balázs Hajgató[2], [1]*Department of Inorganic Chemistry, Institute of Chemistry, Eötvös Loránd University Budapest, Hungary,* [2]*Department SBG, Hasselt University, Belgium*

PP430 **Charge-State Dependent Hydrogen Diffusion on Silicon (001)**
Oliver Warschkow[1], [1]*Centre for Quantum Computer Technology, School of Physics, The University of Sydney, Australia*

PP431 **Exploiting Next-Gen Computers for Computational Quantum Chemistry**
Tirath Ramdas[1], Gregory Egan[1], David Abramson[2], Kim Baldridge[3], [1]*Monash University, Center for Telecommunications and Information Engineering, Australia,* [2]*Monash University, Center for Distributed Systems and Software Engineering, Australia,* [3]*University of Zürich, Organic Chemistry Institute, Switzerland*

PP432 **Thermal Isomerization of 11-cis-Retinal. An Unexpected Manifold**
Carlos Silva Lopez[1], Rosana Alvarez Rodriguez[1], Marta Dominguez Seoane[1], Olalla Nieto Faza[1], Angel R. de Lera[1], [1]*Universidade de Vigo, Spain*

PP433 **Structures and Infrared Spectra of the Topology-Distinct Protonated Water Clusters $H_3O^+(H_2O)_{n-1}$ ($n \leq 6$)**
Maihemutijiang Jieli[1], Misako Aida[1], [1]*Center for Quantum Life Sciences & Graduate School of Science, Hiroshima University, Japan*

PP434 **The Bonding Nature of Dinuclear Cr(II) Complexes. A Theoretical Study with the MRMP2 Method**
Yusaku Kurokawa[1], Yoshihide Nakao[1], Shigeyoshi Sakaki[1], [1]*Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, Japan*

PP435 **Sampling Enhancement for Ab Initio Monte Carlo Calculations of Molecular Clusters**
Akira Nakayama[1], Tetsuya Taketsugu[1], [1]*Division of Chemistry, Graduate School of Science, Hokkaido University, Japan*

PP436 **Complexity under Control: A Theoretical Mechanistic Study of Gold and Platinum Catalyzed Rearrangements**
Olalla Nieto Faza[1], Adán Gonzalez Perez[1], Carlos Silva Lopez[1], Angel R. de Lera[1], [1]*Universidade de Vigo, Spain*

PP437 **Hartree-Fock and Kohn-Sham Response Theory in a Second-Quantization Atomic-Orbital Formalism Suitable for Linear Scaling**
Thomas Kjaergaard[1], Poul Jørgensen[1], Jeppe Olsen[1], Sonia Coriani[2], Trygve Helgaker[3], [1]*Aarhus University Department of Chemistry, Denmark,* [2]*Dipartimento di Scienze Chimiche Universita degli Studi di Trieste, Italy,* [3]*Department of Chemistry, University of Oslo, Norway*

PP438 **Scrutiny of the Mean-Field Approximation to the Two-Electron Spin-Dependent Terms in the Two-Component Pseudo-Relativistic Hamiltonian**
Mojmír Kývala[1], [1]*Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Czech Republic*

PP439 **Theoretical Study of Multi-Nuclear Complexes, $[Pt_2X_4(Me_2pz)_8]$ (X=Ag, Cu, H): Metallophilic LUMO Participation in Strong Luminescence**
Yoshihide Nakao[1], Shigeyoshi Sakaki[1], [1]*Kyoto University, Japan*

PP440 **New Approaches to Large-Scale Multiconfigurational Perturbation Theory Calculations**
Francesco Aquilante[1], Tanya Todorova[1], Laura Gagliardi[1], Björn Olof Roos[2], [1]*Department of Physical Chemistry, Geneva University, Switzerland,* [2]*Department of Theoretical Chemistry, Lund University, Sweden*

PP441 **Spin-Orbit Coupling Effects in Rhenium Tetra-Hydrides**
Shiro Koseki[1], Toshio Asada[1], Taka-aki Hisashima[1], [1]*Department of Chemistry, Osaka Prefecture University, Japan*

PP442 **Chromium-Complexes of Furoxan and Benzofuroxan**
Tibor Pasinszki[1], [1]*Department of Chemistry, Institute of Chemistry, Eötvös Loránd University of Budapest, Hungary*

PP443 **Crowding Effects on Protein Folding: A Binary System Simulation**
Jian Yin[1], Jianwen Jiang[2], Raj Rajagopalan[3], [1]*Singapore-MIT Alliance, Singapore,* [2]*Department of Chemical & Biomolecular Engineering, National University of Singapore, Singapore,* [3]*Singapore-MIT Alliance and Department of Chemical & Biomolecular Engineering, National University of Singapore, Singapore*

PP444 **The Free Energy Change of Glycine Tautomerization in Aqueous Solution**
Miyamoto Hidenori[1], Misako Aida[1], [1]*Center for Quantum Life Sciences & Graduate School of Science, Hiroshima University, Japan*

PP445 **Locating Multiple SCF Solutions: An Approach Inspired by Metadynamics**
Alexander Thom[1], Martin Head-Gordon[1], [1]*University of California, Berkeley, United States*

PP446 **Theoretical Study of the Electric Conductivity in Nb-Doped TiO_2**
Takahiro Suenaga[1], Hideyuki Kamisaka[1], Hisao Nakamura[1], Koichi Yamashita[1], [1]*University of Tokyo, Department of Chemical System Engineering, Japan*

PP447 **Understanding Nucleation Phenomena Near the Spinodal**
Suman Chakrabarty[1], Mantu Santra[1], Prabhakar Bhimalapuram[1], Biman Bagchi[1], [1]*Solid State and Structural Chemistry Unit, Indian Institute of Science, India*

PP448 **DFT and Multinuclear NMR (^{17}O, ^{13}C) Studies of Diazenedicarboxylates and Related Compounds**
Francesca Mocci[1], Michele Usai[1], Giovanni Cerion[1], [1]*Università di Cagliari, Dipartimento di Scienze Chimiche, Italy*

PP449 **The Double-Helical → Ladder Structural Transition in the B-DNA is Induced by a Loss of Dispersion Energy**
Jiří Černý[1], Pavel Hobza[1], [1]*Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Czech Republic*

PP450 **Enzymatic Reaction Mechanism Revealed by Molecular Docking and QM/MM-MD**
Yohsuke Hagiwara[1], Osamu Nureki[2], Masaru Tateno[3], [1]*Graduate School of Pure and Applied Sciences, University of Tsukuba, Japan,* [2]*Institute of Medical Science, University of Tokyo, Japan,* [3]*Center for Computational Sciences, University of Tsukuba, Japan*

PP451 **Density Functional Theory Augmented with an Empirical Dispersion Term – DFT-D – What is the Effect of the Many-Body Terms and Higher Order Contributions to Dispersion?**
Petr Jurecka[1], Mikulas Kocman[1], Pavel Hobza[2], [1]*Palacky University, Czech Republic,* [2]*Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Czech Republic*

PP452 **The Vibrational Band Origins and Potential Energy Surface of Fluorine Isocyanate and its Isomers**
Frank Pickard[1], Yukio Yamaguchi[1], Henry Schaefer III[1], [1]*The University of Georgia, Center for Computational Chemistry, United States*

PP453 **Exploration of Matrix Exponentiation Issues Involved with Non-Reversible Rate Matrices Used in the Modelling of DNA Sequence Evolution**
Harold Schranz[1], [1]*Computational Genomics, John Curtin School of Medical Research, ANU, Australia*

Poster Session 2 – Tuesday September 16 – 5.30-7.30pm

PP454 **The Electronic State of Blue Cu Protein Revealed by the New QM/MM Interface Program**
Takehiro Ohta[1], Yohsuke Hagiwara[2], Masaru Tateno[3], [1]*Institute for Materials Chemistry and Engineering, Kyushu University, Japan,* [2]*Graduate School of Pure and Applied Sciences, University of Tsukuba, Japan,* [3]*Center for Computational Sciences, University of Tsukuba, Japan*

PP455 **Investigation of the Invisible Water Effect for Quantitative Docking Analysis of Protein-Ligand Complexes**
Hitoshi Goto[1], Shigeaki Obata[1], Taku Sugiyama[1], Naofumi Nakayama[1], Kouichi Nishigaki[2], [1]*Toyohashi University of Technology, Japan,* [2]*Saitama University, Japan*

PP456 **Density-Functional Study of Acyclic and Cyclic Phosphoryl Transfer Reactions in Solution: Comparison with Experimental Thio and Isotope Effect Measurements**
Francesca Guerra[1], Jiali Gao[1], Darrin M. York[1], [1]*Department of Chemistry and Supercomputing Institute, University of Minnesota, United States*

PP457 **Photodissociation of the Water Dimer: A 12-D Quasiclassical Study**
Gustavo Avila[1], Geert-Jan Kroes[1], Marc Van Hemert[1], [1]*Leiden University, Leiden Institute of Chemistry, Netherlands*

PP458 **Generator Coordinate Gaussian Basis Sets for the First-Row Atoms: A New Alternative for Pople's and Dunning's Basis Sets**
Moacyr Comar Jr.[1], Francisco Lima[2], Albérico da Silva[3], [1]*Instituto de Ciências Exatas - UFAM, Brazil,* [2]*Instituto de Química de São Carlos - USP, Brazil,* [3]*Instituto de Química de São Carlos - USP, Brazil*

PP459 **Three-Body Corrections to Scaled Opposite Spin Second-Order Møller-Plesset Perturbation Theory**
Robert DiStasio[1], Alex Thom[1], David Casanova[1], Martin Head-Gordon[1], [1]*University of California at Berkeley, Department of Chemistry, United States*

PP460 **Structures of the Mono-Hydrated Guanine-Cytosine Cation**
Heather Jaeger[1], Henry Schaefer III[1], [1]*University of Georgia, Center for Computational Chemistry, United States*

PP461 **Application of Ab Initio DMRG to the Physics of Conjugated π-Electron Systems**
Johannes Hachmann[1], Jonathan J. Dorando[1], Debashree Ghosh[1], Garnet Kin-Lic Chan[1], [1]*Department of Chemistry and Chemical Biology, Cornell University, United States*

PP462 **Molecular Conductance through a Graphene Sheet**
Haitao Wang[1], Garnet Chan[1], [1]*Department of Chemistry and Chemical Biology, Cornell University, United States*

PP463 **The Role of Ligands in Developing Mn_4-based Single-Molecule Magnets and Single-Chain Magnets**
Nguyen Anh Tuan[1], Shin-ichi Katayama[1], Dam Hieu Chi[1], [1]*School of Materials Science, Japan Advanced Institute of Science and Technology, Japan,* [2]*Faculty of Physics, Hanoi University of Science, Viet Nam*

PP464 **Ring Molecules as Basic Modules in Metamaterials?**
Stephan Bernadotte[1,3], Wim Klopper[1,2,3], Ferdiand Evers[1,2], [1]*Institut für Nanotechnologie, Germany,* [2]*Institut für Physikalische Chemie, Universität, Germany,* [3]*Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, Germany*

PP465 **Role of Solvent and Dispersion Forces on the Stability of the DNA Double-Helix**
Martin Kabeláč[1], Pavel Hobza[1], [1]*Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Czech Republic*

PP466 **Design of a Synthetic Catalytic Pore for Cation-Olefin Cyclizations; DFT and MD-Simulations Approach**
Daniel Emery[1], Guillaume Bollot[1], Jiri Mareda[1], [1]*Department of Organic Chemistry, University of Geneva, Switzerland*

PP467 **Projected Entangled Pair States as a Multi-Dimensional Ansatz for Non-Dynamic Correlation in Huge Active Spaces**
Dominika Zgid[1], Garnet Chan[1], [1]*Department of Chemistry and Chemical Biology, Cornell University, United States*

PP468 **Self-Cleavage Catalysis of the Hepatitis Delta Virus Ribozyme Investigated by QM/MM Calculations**
Pavel Banáš[1], Lubomír Rulíšek[2], Daniel Svozil[2], Nils Walter[3], Jiri Šponer[4], Michal Otyepka[1], *[1]Palacky University, Department of Physical Chemistry, Czech Republic, [2]Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Czech Republic, [3]Department of Chemistry, Single Molecule Analysis Group, University of Michigan, United States, [4]Institute of Biophysics, Academy of Science of the Czech Republic, Czech Republic*

PP469 **MOLEONLINE: An Interactive Web-Based Tool to Find and Analyze Molecular Channels, Tunnels and Pores**
Martin Petřek[1], Jaroslav Koča[1], Michal Otyepka[2], *[1]National Centre for Biomolecular Research, Masaryk University, Czech Republic, [2]Department of Physical Chemistry, Palacky University, Czech Republic*

PP470 **A Systematic Study of UVA Chemical Sunscreen Filters**
Jacqueline Cawthray[1], Mark Buntine[1], Stephen Lincoln[1], *[1]Department of Chemistry, University of Adelaide, Australia*

PP471 **Quantum Chemical Simulations of Acetone Adsorption on SWCNTs**
Yoshifumi Nishimura[1], Dmitry Kazachkin[2], Eric Borguet[2], Stephan Irle[1], *[1]Institute for Advanced Research and Department of Chemistry, Nagoya University, Japan, [2]Department of Chemistry, Temple University, United States*

PP472 **Acid-Base Properties of Sterically Demanding Borane–Phosphine Pairs and Implications for Metal-Free Hydrogen Activation**
Tibor András Rokob[1], Andrea Hamza[1], András Stirling[1], Imre Pápai[1], *[1]Chemical Research Center of HAS, Hungary*

PP473 **Different Localization of Protons in the Neutral and Anionic Complexes of Cytosine with Guanine and 8-Oxoguanine**
Iwona Dabkowska[2], Monika Kobylecka[1], Piotr Storoniak[1], Maciej Gutowski[3], Janusz Rak[1], *[1]University of Gdansk, Department of Chemistry, Poland, [2]Free University of Berlin, Physical and Theoretical Chemistry, Germany, [3]Heriot-Watt University, Chemistry-School of Engineering and Physical Sciences, United Kingdom*

PP474 **Theoretical Studies of the CO Adsorption on Pt(111) Surface Using Cluster Models**
Yu-Wei Huang[1], Ting-Yi Chou[1], Yan-Yu Chen[1], Shyi-Long Lee[1], *[1]Department of Chemistry and Biochemistry, National Chung Cheng University, Taiwan*

PP475 **In Silico and In Vitro Mutagenesis of PA-IIL Lectin – Correlation with Structure-Function Analysis**
Jan Adam[1], Martina Pokorna[1], Zdenek Kriz[1], Martin Prokop[1], Jaroslav Koča[1], Michaela Wimmerova[1], *[1]Masaryk University, National Centre for Biomolecular Research, Czech Republic*

PP476 **Theoretical Study of the Minor Channel Forming HNO_3 in the HO_2 + NO Reaction**
Marie-Therese Rayez[1], Jean-Claude Rayez[1], *[1]Universite Bordeaux1-ISM-groupe THEO, France*

PP477 **Solvent Effects for the Interaction of Adenine Adducts with Thymine**
Prabhat K. Sahu[1], Yu-Wei Huang[1], Shyi-Long Lee[1], *[1]Department of Chemistry and Biochemistry, National Chung Cheng University, Taiwan*

PP478 **Ab Initio Molecular Energies by Fragmentation: A Feasible Strategy for Non-Bonded Interactions**
M. A. Addicoat[1], M. A. Collins[1], *[1]Research School of Chemistry, Australian National University, Australia*

PP479 **Agonist Binding at the Calcium Sensing Receptor: A Computational Approach**
Susan Corley[1], Hoi-Ming Chan[1], Meredith Jordan[1], *[1]School of Chemistry, The Univeristy of Sydney, Australia*

PP480 **Performance of Density Functionals in a QM and QM/MM study of the Catalytic Mechanism of β-Galactosidase**
Pedro Alexandrino Fernandes[1], Natércia Brás[1], Sara Moura-Tamames[1], Ramos Maria[1], *[1]Requimte/Faculty of Sciences, University of Porto, Portugal*

PP481 **Molecular Modelling of Hydrotalcite Layered Double Hydroxide Structures Intercalcated with Transition Metal Oxide Anions**
Vinutha Murthy[1], Howard D Smith[2], *[1]Charles Darwin University, School of Environmental & Life Sciences, Australia, [2]Curtin University of Technology, Nanochemistry Research Institute, Australia*

Poster Session 2 – Tuesday September 16 – 5.30-7.30pm

PP482 **Computational Studies on the Thermal Fragmentation Reactions of 1,4,2-Oxathiazole Derivatives – A Convenient Synthesis of Isothiocyanates**
Robert O'Reilly[1], Leo Radom[1], *[1]School of Chemistry, The University of Sydney, Australia*

PP483 **Potential Energy Hypersurface for the Methane Radical Cation**
Lucas D. Speakman[1], Justin M. Turney[1], Henry F. Schaefer III[1], *[1]University of Georgia, Center for Computational Chemistry, United States*

PP484 **A Computational Study of Substrate Mechanism of Pyruvate-Formate Lyase**
Karmen Condic-Jurkic[1], V. Tamara Perchyonok[2], Hendrik Zipse[3], David M. Smith[1], *[1]Rudjer Boškovic Institute, Centre for Computational Solutions in the Life Sciences, Croatia, [2]Monash University, School of Chemistry, Australia, [3]Ludwig-Maximilians-Universität, Department Chemie und Biochemie, Germany*

PP485 **The Enthalpy of Formation and Anharmonic Force Field for Diacetylene**
Andrew Simmonett[1], Wesley Allen[1], Henry F. Schaefer III[1], *[1]Center for Computational Chemistry, University of Georgia, United States*

PP486 **Perturbative Triples Correction for State-Specific Multireference Coupled Cluster**
Francesco A. Evangelista[1], Wesley D. Allen[1], Henry F. Schaefer III[1], *[1]Center for Computational Chemistry, University of Georgia, United States*

PP487 **A Theoretical Study on the S_1/S_2 Conical Intersection Along the Amino Inversion Coordinate of Aminonaphthalene**
Masayuki Nakagaki[1], Haruyuki Nakano[1], *[1]Department of Molecular Chemistry, Graduate School of Sciences, Kyushu University, Japan*

PP488 **Non Specific Binding of Positron Emission Tomography (PET) Ligands as Seen from an Ab Initio Computational Study**
Lula Rosso[1], Antony Gee[2], Ian Gould[1], *[1]Department of Chemistry, Imperial College London, United Kingdom, [2]Clinical Imaging Centre, United Kingdom*

PP489 **Laser Control of Photoassociation in Diatomic Molecules**
Kiyoshi Nishikawa[1], Masatoshi Sano[1], Atsuhito Tawada[1], Shunichi Taniguchi[1], Kimikazu Sugimori[2], Hidemi Nagao[1], *[1]Kanazawa University, Division of Mathematical and Physical Science, Japan, [2]Kinjo University, Japan*

PP490 **Photochemistry of Fischer Carbene Complexes**
Israel Fernández[1], Miguel A. Sierra[1], *[1]Dpto. de Química Orgánica, Universidad Complutenses de Madrid, Spain*

PP491 **Interaction of Roxithromycin with 50S Large Ribosomal Subunit: Molecular Dynamics Simulation**
Wai Keat Yam[1], Habibah A Wahab[1], *[1]Pharmaceutical Design and Simulation Laboratory, School of Pharmaceutical Sciences, Universiti Sains Malaysia, Malaysia*

PP492 **Computational Studies on Bimetallic Clusters**
Ying-Chan Lin[1], Li-Feng Cui[2], Lai-Sheng Wang[3], Dage Sundholm[1], *[1]Department of Chemistry, University of Helsinki, Finland, [2]Department of Physics, Washington State University, United States, [3]Sciences Laboratory and Chemical Sciences Division, Pacific Northwest National Laboratory, United States*

PP493 **Are Isomers of the Vinyl Cyanide Ion Missing Links for Interstellar Pyrimidine Formation?**
Partha P. Bera[1], Timthy J. Lee[1], Henry F. Schaefer III[2], *[1]NASA Ames Research Center, Space Science and Astrobiology, United States, [2]University of Georgia, Center for Computational Chemistry, United States*

PP494 **Molecular Shape Analysis Using Ion Probes and its Applications**
Manabu Sugimoto[1], *[1]Kumamoto University, Japan*

PP495 **The Hydrogen Bond in Transmembrane Proteins**
Dah-Yen Yang[1], *[1]Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan*

PP496 **Molecular Dynamics of Hydrogen Bonds in Protein-D_2O**
Sheu-Yi Sheu[1], *[1]Faculty of Life Sciences and Institute of Genome Sciences, National Yang-Ming University, Taiwan*

PP497 **Atomistic Modelling of Soot Particles and of their Interaction with Surrounding Molecules**
J C Rayez[1], M T Rayez[1], B Collignon[2], S Picaud[2], P N M Hoang[2], *[1]Universite Bordeaux1, Institut des Sciences Moleculaires (ISM), CNRS, France, [2]Université de Franche-Comté, Institut UTINAM, CNRS, France*

PP498 **Phosphotriesterase-Catalyzed Hydrolysis of Toxic Organophosphorus Compounds: Modelling of the Enzyme-Substrate Complex**
Edyta Dyguda-Kazimierowicz[1], Jolanta Zurek[2], Adrian Mulholland[2], W. Andrzej Sokalski[1], Jerzy Leszczynski[3], *[1]Institute of Physical and Theoretical Chemistry, Wroclaw University of Technology, Poland, [2]Centre for Computational Chemistry, School of Chemistry, University of Bristol, United Kingdom, [3]Computational Center for Molecular Structure and Interactions, Jackson State University, United States*

PP499 **Combining the Time Reversal Symmetry with Point Group Symmetry in Relativistic Molecular Calculations**
Daoling Peng[1], Kimihiko Hirao[1], *[1]Department of Applied Chemistry, The University of Tokyo, Japan*

PP500 **The FMO/EFP Energy Gradient and its Applications to Solvated Peptide Molecules**
Takeshi Nagata[1], Dmitri Fedorov[1], Mark Gordon[2], Kazuo Kitaura[3], *[1]AIST, Japan, [2]Iowa State University, United States, [3]Kyoto University, Japan*

PP501 **Dense Packing of Binary Spheres**
Gavin Marshall[1], Jonathan Kummerfeld[1], Toby Hudson[1], Peter Harrowell[1], *[1]School of Chemistry, The University of Sydney, Australia*

PP502 **Spectroscopic and Electric Properties of Tungsten Carbide**
Ivan Černušák[1], Miroslav Urban[1], Vladimír Kellö[1], Martina Čurkovičová[1], *[1]Department of Physical and Theoretical Chemi*stry, *Comenius University, Slovakia*

PP503 **Acyl Radical Addition to Pyridine: Multiorbital Interactions**
Ruth Amos[1,2], Carl Schiesser[2,3,4], Jason Smith[1,2], Brian Yates[1,2], *[1]School of Chemistry, University of Tasmania, Australia, [2]ARC Centre of Excellence for Free-Radical Chemistry and Biotechnology, Australia, [3]School of Chemistry, The University of Melbourne, Australia, [4]Bio21 Molecular Science and Biotechnology Institute , The University of Melbourne, Australia*

PP504 **Selenium in Pyrite – Why is the XANES Spectrum of Iron Selenide not Observed?**
Nicholas Lambropoulos[1], Ken Riley[1], David French[1], *[1]CSIRO Energy Technology, Australia*

PP505 **Density Matrix Renormalization Group Response Theory**
Jon Dorando[1], Johannes Hachmann[1], Garnet Chan[1], *[1]Cornell Chemistry and Chemical Biology, Cornell University, United States*

PP506 **Things You Take For Granted in Closed-Shell MP2: The Subtleties of ROHF References in F12 Methods**
Jeremiah Wilke[1], Henry F. Schaefer III[1], Wesley Allen[1], *[1]Center of Computational Chemistry, University of Georgia, United States*

PP507 **How Strong Is It? The Interpretation of Force and Compliance Constants as Bond Strength Descriptors**
Kai Brandhorst[1], Jörg Grunenberg[1], *[1]Technische Universität Braunschweig, Institut für Organische Chemie, Germany*

PP508 **Efficient Computation of Inverse Hessians and Compliance Matrices in Redundant Internal Coordinates from Cartesian Hessians**
Kai Brandhorst[1], Jörg Grunenberg[1], *[1]Technische Universität Braunschweig, Institut für Organische Chemie, Germany*

PP509 **Quantized-Liquid Density Functional Theory of Hydrogen Adsorption in Nano-Porous Substrates**
Serguei Patchkovskii[1], Thomas Heine[2], *[1]NRC Canada, Canada, [2]Jacobs University, Germany*

PP510 **XUV Probing of a Recollision Electron Wavepacket: An Attosecond Electron Microscope**
Olga Smirnova[1], Serguei Patchkovskii[1], Michael Spanner[1], *[1]NRC Canada, Canada*

PP511 **QSPR Studies on the Prediction of Physicochemical Properties of High Energetic Materials: Melting Points**
Chan Kyung Kim[1], Soo Gyeong Cho[2], In Suk Han[1], Junxian Chen[1], Hyok Yoon[1], Hai Whang Lee[1], Bon-Su Lee[1], *[1]Inha University, Department of Chemistry, Korea, Republic of, [2]Agency for Defence Development, Korea, Republic of*

Poster Session 2 – Tuesday September 16 – 5.30-7.30pm

PP512 **Theoretical Studies on Nucleophilic Substitution Reactions of Acetyl and Thioacetyl Halides with NH_3 in the Gas Phase and in Aqueous Solution**
In Suk Han[1], Chang Kon Kim[1], Hyok Yoon[1], Hai Whang Lee[1], Chan Kyung Kim[1], *[1]Inha University, Department of Chemistry, Korea, Republic of*

PP513 **Effects of Basis Set Superposition Error on Optimized Geometries and Energies of an Organo-Alkali Metal Cation and its Halide Complexes**
Chang Kon Kim[1], In Suk Han[1], Hyok Yoon[1], Jongok Won[2], Chan Kyung Kim[1], *[1]Inha University, Department of Chemistry, Korea, Republic of, [2]Sejong University, Department of Applied Chemistry, Korea, Republic of*

PP514 **Theoretical Study of the Acid-Base Properties of Piroxicam and Isoxicam**
Marco Antonio Franco-Pérez[1], Rosario Moya-Hernández[1], Rodolfo Gómez-Balderas[1], *[1]FESC-Cuautitlán, UNAM, Departamento de Química, México*

PP515 **Accurate Hartree-Fock Calculation Using Perturbation Theory**
Jia Deng[1], Peter Gill[1], *[1]Research School of Chemistry, Australian National University, Australia*