POSTERS

Poster Session and Mixer 1

Time: 18:15 - 20:15
Date: Monday September 30, 2019
Location: Upper ABS Foyer

P001

A Molecular Simulation Study of Carbon Dioxide Adsorption in Two Interpenetrated Metal-Organic Frameworks: LMOF-201 and 202

Ankit Agrawal[1], Mayank Agrawal[2], Donguk Suh[1], Yunsheng Ma[3], Ryotaro Matsuda[3], Wei-Lun Hsu[1], Hirofumi Daiguji[1]
[1]University of Tokyo, Tokyo, Japan. [2]Georgia Institute of Technology, Atlanta, USA. [3]Nagoya University, Nagoya, Japan

P002

Investigating Luminescent Metal Complexes using Computational Methods

Johnny Agugiaro, David Wilson
La Trobe University, Melbourne, Australia

P003

Theoretical Investigation of Ring-Expansion of N-Heterocyclic Carbenes (NHCs) Containing C, P, O, S Heteroatoms

Khalidah Al-Furaiji, David Wilson
La Trobe Institute for Molecular Science, Melbourne, Australia

P004

Roby-Gould Bond Indices as a Tool in Chemistry

Khidhir Alhameedi
School of Molecular Sciences, The University of Western Australia, Perth, Australia

P006

Toroidal States in an Isosceles Spin Triangle Without Spin-Orbit Coupling: Applications in a Molecular Spintronics Device

Jared Ashtree, Shashank Rao, Alessandro Soncini
University of Melbourne, Parkville, Australia

P007

Valence and Core Electron Spectroscopy for the Conformational Study of Bio-active Pyridine Derivatives

Fred Backler[1], Hanan Sa'adeh[2,3], Kevin Prince[3], Feng Wang[1]
[1]Swinburne University of Technology, Melbourne, Australia. [2]The University of Jordan, Amman, Jordan. [3]Elettra Sincrotrone, Trieste, Italy

P008

Effect of Ca-Dopant on Lithium Ion Conductivity in $Li_7P_3S_{11}$ and Li_3PS_4 Solid Electrolytes

Ardeshir Baktash[1], Debra Searles[1,2]
[1]Centre for Theoretical and Computational Molecular Science, Australian Institute for Bioengineering and Nanotechnology, the University of Queensland, Queensland , Brisbane, Australia. [2]School of Chemistry and Molecular Biosciences, the University of Queensland, Queensland , Brisbane, Australia

P009

Towards an Understanding of Field Effects in the G-Quadruplex/Hemin DNAzyme Peroxidation Catalysis.

Clare Birch, Meredith Jordan
The University of Sydney, Sydney, Australia

P010

Theoretical Progress Towards pH-Switchable Electrostatic Catalysis

Mitchell Blyth, Michelle Coote
Research School of Chemistry, Australian National University, Canberra, Australia

P011

Fine Tuning of Ligand Field Splitting in Iron(II) Complexes

Luca Bondi[1,2], Federico Totti[2], Paul Jerabek[3], Anna Garden[1], Sally Brooker[1]
[1]University Of Otago, Dunedin, New Zealand. [2]University Of Florence, Florence, Italy. [3]Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany

P012

Microscopic Mechanism of SEI Film Formation in Highly Concentrated Electrolytes Based on Nonflammable Trimethyl Phosphate Solvent

Amine Bouibes[1], Norio Takenaka[2], Soumen Saha[3], Masataka Nagaoka[1]
[1]Nagoya University, Nagoya, Japan. [2]University of Tokyo, Tokyo, Japan. [3]Kyoto University, Nagoya, Japan

P013

On the Application of the Hubbard-U Correction in Modelling Semiconductors for Solar Water Splitting

Joshua Brown, Alister Page
The University of Newcastle, Newcastle, Australia

P014

Effect of Magnetic Anisotropy on Direct Chiral Discrimination in Paramagnetic NMR Spectroscopy

Simone Calvello[1,2], Alessandro Soncini[1]
[1]The University of Melbourne, Melbourne, Australia. [2]Australia's Nuclear Science and Technology Organisation, Sydney, Australia

P015

The Full Potential Energy Surface for N-H Tautomerisation in Free-Base Porphyrin

Peter Canfield[1,2,3], Jeffrey Reimers[4,3], Maxwell Crossley[1]
[1]The School of Chemistry, University of Sydney, Sydney, Australia. [2]ORAinnova, Sydney, Australia. [3]International Centre for Quantum and Molecular Structures, Shanghai University, Shanghai, China. [4]University of Technology Sydney, Sydney, Australia.

P016

Long-Range Corrected Double Hybrid Density Functionals Optimised for Electronic Excitations

Marcos Casanova-Páez, Lars Goerigk
The University of Melbourne, Melbourne, Australia

P017

Towards an Accurate Description of Solvent Effects

Junbo Chen[1], Yihan Shao[2], Bun Chan[3], Junming Ho[1]
[1]University of New South Wales, Sydney, Australia. [2]University of Oklahoma, Norman, USA.
[3]Nagasaki University, Nagasaki, Japan

P018

Molecular Vibrational Spectroscopy Study by Path Integral Liouville Dynamics

Zifei Chen, Zhijun Zhang, Xinzijian Liu, Kangyu Yan, Haifeng Zheng, Jian Liu
Institute of Theoretical and Computational Chemistry, College of Chemistry and Molecular Engineering, Peking University, Beijing, China

P019

Computational Insights into the Role of BINOL-Derived Catalysts in Asymmetric Nazarov Cyclisations

Yuk Ping Chin, Elizabeth Krenske
[1]School of Chemistry and Molecular Biosciences, The University of Queensland, Australia

P020

An In-Silico Investigation of Menthol Metabolism

Taweetham Limpanuparb, Wanutcha Lorpaiboon, Kridtin Chinsukserm
Mahidol University, Salaya, Thailand

P021

Recent Development of Automatized Density-Functional Tight-Binding Parameterization for Metal-Containing Systems

Chien-Pin Chou[1], Aditya Sakti[2], Hiromi Nakai[1,2,3]
[1]Waseda Research Institute for Science and Engineering (WISE), Waseda University, Tokyo, Japan.
[2]Element Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University, Kyoto, Japan.
[3]Department of Chemistry and Biochemistry, School of Advanced Science and Engineering, Waseda University, Tokyo, Japan

P022

Collisional Energy Transfer Between Hot CH_3CHO/CH_2CHOH and N_2

Maggie Corrigan, Isabella Russell, Meredith Jordan
School of Chemistry, the University of Sydney, Sydney, Australia

P023

Predicting NMR Spectra Using Mixed Pseudoramp-Gaussian Basis Sets

Claudia Cox[1], Juan Camilo Trujillo[2,1], Laura McKemmish[1]
[1]UNSW, Sydney, Australia. [2]Universidad Icesi, Cali, Colombia

P024

fragHAR: Towards Ab Initio Quantum Crystallographic X-Ray Structure Refinement for Polypeptides and Proteins

Justin Bergmann[1], Max Davidson[2], Esko Oksanen[3], Ulf Ryde[1], Dylan Jayatilaka[2]
[1]Lund University, Lund, Sweden. [2]University of Western Australia, Perth, Australia. [3]European Spallation Source, Lund, Sweden

P025

Electronic Structure Understanding of the Mechanically Induced Selectivity in Acid Catalyzed Chitin Hydrolysis

Danjo De Chavez[1], Horikazu Kobayashi[2], Atsushi Fukuoka[2], Jun-ya Hasegawa[2]
[1]Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo, Japan. [2]Institute for Catalysis, Hokkaido University, Sapporo, Japan

P026

Studies of Peroxide Intermediate Structure and Mechanism of the Aryl Nitration Reaction in Nonheme N-Oxygenase CmlI – A Theoretical Study

Salai Kalaiselvi Dhanasekaran, Senthilnathan Dhurairajan
Centre for Computational Chemistry, CRD, PRIST Deemed to be University, Thanjavur, India

P027

Computational Design of Highly Activating Ligands for Atom-Transfer Radical Polymerisation

Phuong Doan, Benjamin Noble, Alfred Fung, Michelle Coote
ARC Centre of Excellence for Electromaterials Science, Research School of Chemistry, Australian National University, Canberra, Australia

P028

Effect of Liquid Phase on Heterogeneous Catalytic Reactions

Swarit Dwivedi[1], Samir Mushrif[2], Alan Chaffee[1], Akshat Tanksale[1]
[1]Monash University, Melbourne, Australia. [2]University of Alberta, Edmonton, Canada

P029

Exploring the Structure and Mechanism of Transport of the Human Sodium Proton Exchanger Isoform One (NHE1)

Nehad El Salamouni[1,2,3], Michael Kelso[1,2,3], Haibo Yu[1,2,3]
[1]School of Chemistry and Molecular Bioscience, , University of Wollongong , Wollongong, Australia. [2]Molecular Horizons, University of Wollongong, Wollongong, Australia. [3]Illawarra Health and Medical Research Institute, Wollongong, Australia

P030

Molecular Dynamics Simulations of Specific Ion Effects at Interfaces

Gareth Elliott, Grant Webber, Erica Wanless, Alister Page
University of Newcastle, Callaghan, Australia

P031

Predicting the Basicity of *N*-Heterocyclic Carbenes

Alicia Evans, Jason Harper, Junming Ho
UNSW, Sydney, Australia

P032

Accurate Approach in Simulating the Electronic Absorption Cross Section of Small to Medium Molecules

Sara Farahani, Joseph Lane
University of Waikato, Hamilton, New Zealand

P033

Energy-Based Automatic Fragmentation in the Linear-Scaling Divide-and-Conquer Electron Correlation Calculations

Toshikazu Fujimori[1], Masato Kobayashi[2,3,4], Tetsuya Taketsugu[1,2,3,4]
[1]Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo, Japan. [2]Faculty of Science, Hokkaido University, Sapporo, Japan. [3]WPI-ICReDD, Hokkaido University, Sapporo, Japan. [4]ESICB, Kyoto University, Kyoto, Japan

P034

Machine Learning Study for Optimization of Reaction Conditions Including Discrete Variables with Small Number of Experiments

Mikito Fujinami[1], Hiroki Maekawara[1], Junji Seino[2,3], Hiromi Nakai[1,2,4]
[1]Department of Chemistry and Biochemistry, School of Advanced Science and Engineering, Waseda University, Tokyo, Japan. [2]Waseda Research Institute for Science and Engineering, Waseda University, Tokyo, Japan. [3]PRESTO, Japan Science and Technology Agency, Saitama, Japan. [4]Element Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University, Kyoto, Japan

P035

Mechanism and Optimisation of Nitroxide Mediated Photopolymerisation

Melinda Fule[1], Nicholas Hill[1,2], Michelle Coote[1,2]
[1]Australian National University, Canberra, Australia. [2]ARC Centre of Excellence for Electromaterials Science, Wollongong, Australia

P036

Parallel MP2 by Quadrature

Giuseppe Barca, Simon McKenzie, Andrew Gilbert, Nathaniel Bloomfield, Peter Gill
Australian National University, Canberra, Australia

P038

Decomposing Specific-Ion Interactions

Kasimir Gregory, Erica Wanless, Grant Webber, Alister Page
The University of Newcastle, Callaghan, Australia

P039

Molecular Modelling of Non-Ionic Surfactant ($C_{12}E_6$) Aqueous Phase Behaviour

Amali Guruge[1], Dallas Warren[2], Colin Pouton[2], David Chalmers[1]
[1]Medicinal Chemistry, Monash Institute of Pharmaceutical Sciences, Monash University, 381 Royal Parade, Parkville, Victoria 3052, Australia. [2]Drug Delivery, Disposition and Dynamics, Monash Institute of Pharmaceutical Sciences, Monash University, 381 Royal Parade, Parkville, Victoria 3052, Australia

P040

Influence of Sugar and Bases on the Stretching Vibrations of PO_2^- of DNA: A Computational Study with FMO/FDD.

Eunice Gwee[1,2,3], Kamila Kochan[1,3], Glen Deacon[1], Bayden Wood[1,3], Ekaterina Izgorodina[1,2]
[1]Monash University, Melbourne, Australia. [2]Monash Computational Chemistry Group, Melbourne, Australia. [3]Centre of Biospectroscopy, Melbourne, Australia

P041

Theoretical Study of Ni Catalysts for H_2 Oxidation and Production via the Minimum Energy Intersystem Crossing Point

Sarinya Hadsadee[1], Manussada Ratanasak[2], Siriporn Jungsuttiwong[1], Jun-ya Hasegawa[2]
[1]Ubon Ratchathani University, Ubon Ratchathani, Thailand. [2]Hokkaido University, Hokkaido, Japan

P042

Electronic Transport Investigation of Redox-Switching Azulenequinones/Hydroquinones via First-Principles Studies

El-Abed Haidar[1], Sherif Tawfik[2], Catherine Stampfl[1], Kimihiko Hirao[3], Kazunari Yoshizawa[4], Safinaz El-Demerdash[5], Takahito Nakajima[3], Ahmed El-Nahas[3,4,5]
[1]School of Physics, The University of Sydney, Sydney, New South Wales 2006, Australia, Sydney, Australia. [2]School of Science, RMIT University, GPO Box 2476 Melbourne, Victoria 3001 Australia, Melbourne, Australia. [3]RIKEN, Advanced Institute for Computational Science, 7-1-26 Minatojima-minami, Chuo, Kobe 650-0047, Japan, Kobe, Japan. [4]Institute for Materials Chemistry and Engineering, Kyushu University, Nishi-ku, Fukuoka 819-0395, Japan, Fukuoka , Japan. [5]Chemistry Department, Faculty of Science, Menoufia University, Shebin El-Kom 32512, Egypt, Shebin El-Kom, Egypt

P043

Normal Mode Analysis for Vibrational Motions in Liquid Water

Zheng Haifeng, Yi Shasha
Peking University, Beijing, China

P044

Transport Properties of Ionic Liquids from MD Simulations with a Self-Consistent Atomic Charge Determination

Lukman Hakim[1,2,3], Yoshiki Ishii[2], Nobuyuki Matubayasi[2]
[1]Elements Strategy Initiative for Catalysts and Batteries, Kyoto University, Kyoto, Japan. [2]Graduate School of Engineering Science, Osaka University, Osaka, Japan. [3]Department of Chemistry, Brawijaya University, Malang, Indonesia

P045

Ab Initio Examination of Nitrogen Gas Solubility in Fluorinated Ionic Liquid Clusters

Peter Halat, Douglas MacFarlane, Katya Pas
Monash University, Clayton, Australia

P046

Assessing Noncovalent Interactions in Electronic Excited States

Amy Hancock, Lars Goerigk
University of Melbourne, Melbourne, Australia

P047

Finding and Analyzing Interfacial Amorphous Carbon Structures in CNT-Based Functional Materials by Artificial Force Induced Reaction Method

Taisuke Hasegawa[1], Makito Takagi[2], Yosuke Sumiya[3], Satoshi Maeda[3,1]
[1]NIMS, Tsukuba, Japan. [2]Yokohama City University, Yokohama, Japan. [3]Hokkaido University, Sappro, Japan

P048

Understanding the Extent of Ionicity in Diamine Protic Ionic Liquids

Fairuz Hashim[1], Steven Pas[2], Douglas MacFarlane[1], Ekaterina Izgorodina[1]
[1]Monash University, Melbourne, Australia. [2]Defence Science and Technology Organisation, Melbourne, Australia

P049

Tuning of the Dielectric Constant to Correct for Delocalisation Error: Development and Preliminary Testing of a Novel Computational Method

Luke Hemmingsen[1], Oliver Hervir[1], Stephen Dale[1,2]
[1]Australian National University, Canberra, Australia. [2]University of Sydney, Sydney, Australia

P050

Internal Oriented Electric Fields as a Strategy for Selectively Modifying Photochemical Reactivity

Nicholas Hill[1,2], Michelle Coote[1,2]
[1]Australian National University, Canberra, Australia. [2]ARC Centre of Excellence for Electromaterials Science, Wollongong, Australia

P051

Importance of Li Distribution on High Li Conductivity in $Li_x(Ge,P)_3S_{12}$

Yoyo Hinuma[1,2], Takeshi Yajima[3], Satoshi Hori[4], Rui Iwasaki[3], Zenji Hiroi[3], Ryoj Kanno[4]
[1]Chiba University, Chiba, Japan. [2]National Institute for Materials Science, Tsukuba, Japan. [3]University of Tokyo, Kashiwa, Japan. [4]Tokyo Institute of Technology , Yokohama, Japan

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P052

Effect of Protonation on the Reaction Mechanism of Fragmentation and 1,3-Rearrangement *via* Breslow Intermediates

Ming-Hsiu Hsieh[1,2], Jen-Shiang Yu[1,2,3]
[1]Department of Biological Science and Technology, National Chiao Tung University, Hsinchu, Taiwan. [2]Institute of Bioinformatics and Systems Biology, National Chiao Tung University, Hsinchu, Taiwan. [3]Center for Intelligent Drug Systems and Smart Bio-devices (IDS2B), National Chiao Tung University, Hsinchu, Taiwan

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P053

Without Compromising Efficiency and Accuracy: Solving the Nuclear Schrödinger Equation Using Path Integral Monte Carlo Simulation with Modified Shepard Interpolation

Gavin Huang, Meredith Jordan
The University of Sydney, Sydney, Australia

P054

Molecular Spintronics with Single-Molecule Magnets Under Irradiation

Kieran Hymas, Alessandro Soncini
The University of Melbourne, Melbourne, Australia

P055

A Systematic Study on Bond Activation Energies of NO, N_2, and O_2 Catalyzed by Eight Transition Metal Hexamers

Tomoya Ichino[1], Satoshi Maeda[1,2,3]
[1]Department of Chemistry, Faculty of Science, Hokkaido University, Sapporo, Japan. [2]Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University, Sapporo, Japan. [3]Research and Services Division of Materials Data and Integrated System (MaDIS), National Institute for Materials Science (NIMS), Tukuba, Japan

P056

Key Factor of the S_0/S_1 Minimum Energy Conical Intersection

Mayu Inamori[1], Yasuhiro Ikabata[2], Takeshi Yoshikawa[2], Hiromi Nakai[1,2,3]
[1]Department of Chemistry and Biochemistry, Waseda University, Tokyo, Japan. [2]WISE, Waseda University, Tokyo, Japan. [3]ESICB, Kyoto University, Kyoto, Japan

P057

The Production of Formic Acid and Formaldehyde From CO_2 Using Boron-Doped Diamond: A Theoretical Study

Yuwanda Injongkol[1,2], Siriporn Jungsuttiwong[1], Alejandro Montoya[2]
[1]Department of Chemistry, Faculty of Science, Ubon Ratchathani University, Ubon Ratchathani, Thailand. [2]School of Chemical and Biomolecular Engineering, The University of Sydney, Sydney, Australia

P058

The Role of Solvation in Predicting Protein–Ligand Binding Affinities: Validating the Automated Topology Builder

Kasey Ireland, Nicole Wheatley, Martin Stroet, Alan Mark
University of Queensland, Brisbane, Australia

P059

An Exploration of Bifurcation on a Reaction Route Network of a Diels–Alder Reaction Based on the AFIR Method

Takuma Ito[1], Yu Harabuchi[2,3,4], Satoshi Maeda[2,4,5]
[1]Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo, Japan. [2]Department of Chemistry, Faculty of Science, Hokkaido University, Sapporo, Japan. [3]JST, PRESTO, Saitama, Japan. [4]WPI-ICReDD, Sapporo, Japan. [5]NIMS, Tsukuba, Japan

P060

Investigating the Mechanism of High Performing Dielectric Materials

Lilit Jacob, Terry Frankcombe
UNSW, Canberra, Australia

P061

Identifying Binding Modes of Neurosteroids at an Intra-Subunit Pocket on $GABA_A$ Receptors

Tian Jiang[1,2], Ali Kusay[1,2], Thomas Balle[1,3]

[1]Sydney School of Pharmacy, Faculty of Medicine and Health, The University of Sydney, Sydney, Australia. [2]Brain and Mind Centre, The University of Sydney, Sydney, Australia. [3]Brain and Mind, The University of Sydney Centre, Sydney, Australia

P062

Implications of Hybrid Organic–Inorganic Functionalized Dodecaborane Dianions in Lithium and Magnesium Ion Batteries

Meenakshi Joshi[1,2], Tapan Ghanty[1,2]

[1]Homi Bhabha National Institute, Mumbai, India. [2]Theoretical Chemistry Section, Chemistry Group, Bhabha Atomic Research Centre, Mumbai, India

P063

Computational Insights into the Origin of Enantioselectivity in a Palladium Catalyzed Dynamic Kinetic Asymmetric Transformation of Racemic Biaryls

Surya K, Raghavan Sunoj

Indian Institute of Technology Bombay, Mumbai, India

P064

Stabilising Molecular Fragments of Group 13, 15 Heteronuclear Diatomics

Aishvaryadeep Kaur, David Wilson

La Trobe University, Melbourne, Australia

P065

Examination of Statistical Methods for Analyzing Fragment Molecular Orbital Calculation Results on Ligand-Protein Interactions.

Yusuke Kawashima[1], Nanami Mori[1], Hirotomo Moriwaki[2], Norihito Kawashita[3], Yu-Shi Tian[1], Tatsuya Takagi[1]

[1]Graduate School of Pharmaceutical Sciences, Osaka University, Suita, Japan. [2]RIKEN Center for Biosystems Dynamic Research, Yokohama, Japan. [3]Faculty of Science and Engineering, Kindai University, Higashi Osaka, Japan

P066

HACA Accelerated: The Role of the Submerged Barrier in the Rate of Radical–Acetylene Addition Reactions

Patrick Kelly[1], Oisin Shiels[1], Aislinn Turner[1], Brett Burns[1], Cameron Bright[1], Stephen Blanksby[2], Gabriel da Silva[3], Adam Trevitt[1]
[1]University of Wollongong, Wollongong, Australia. [2]Queensland University of Technology, Brisbane, Australia. [3]University of Melbourne, Melbourne, Australia

P067

Control of Ziegler–Natta Catalyst Activity by the Structural Design of External Donor

Vikas Khatri[1], Gurmeet Singh[2], Hemant Kashyap[1]
[1]Indian Institute of Technology, Delhi, India. [2]R&D Center, IndianOil Corporation Ltd, Faridabad, India

P068

Size-Dependent Level Alignment Between Anatase and Rutile TiO_2 Nanoparticles

Kyoung Chul Ko
Chonnam National University, Gwangju, Korea, Republic of

P069

Practical Excited-State Simulation of Thousands of Atoms

Nana Komoto[1], Takeshi Yoshikawa[2], Junichi Ono[2], Yoshifumi Nishimura[2], Hiromi Nakai[1,2,3]
[1]Department of Chemistry and Biochemistry, Waseda University, Tokyo, Japan. [2]WISE, Waseda University, Tokyo, Japan. [3]ESICB, Kyoto University, Kyoto, Japan

P070

Catalysis by Pure Graphene - From Supporting Actor to Protagonist through π–π Interactions

Asja Kroeger, Amir Karton
The University of Western Australia, Perth, Australia

P071

Role of Atmospheric Molecular Clusters in the Atmosphere

Jakub Kubečka, Theo Kurtén, Hanna Vehkamäki
University of Helsinki, Helsinki, Finland

P072

Towards Selective nAChR Therapeutics: Identifying the Binding Mode of CMPI and NS9283 in α4β2 nAChRs

Ali Kusay[1,2], Thomas Balle[1,2]
[1]Sydney School of Pharmacy, Faculty of Medicine and Health, The University of Sydney, Sydney, Australia. [2]Brain and Mind Centre, The University of Sydney, Sydney, Australia

P073

Calculating the Exact Ground-State Wave Function of Two-Electron Atoms via Analytic Perturbation Theory

Johanna Langner, Henryk Witek
National Chiao Tung University, Hsinchu, Taiwan

P074

Insights into $MoTe_2$ Intrinsic Defects from Ab Initio Calculations

Martina Lessio[1], Alexander Kerelsky[2], Abhay Pasupathy[2], David Reichman[2]
[1]University of Sydney, Sydney, Australia. [2]Columbia University, New York, USA

P075

Scaffold-Based Molecular Design Using Graph Generative Model

Jaechang Lim, Sang-Yeon Hwang, Seungsu Kim, Seokhyun Moon, Woo Youn Kim
KAIST, Daejeon, Korea, Republic of

P076

Investigating the Effects of Membrane Lipid Composition on Neurotransmitter Transport Function

Yiechang Lin, Katie Wilson, Megan O'Mara
Australian National University, Canberra, Australia

Poster Session and Mixer 2

Time: 18:00 - 20:00
Date: Tuesday October 1, 2019
Location: Upper ABS Foyer

P077

Finding Electrons: Transforming Chemical Thought by Analysing Wavefunctions

Yu Liu
The Univeristy of New South Wales, Sydney, Australia

P078

Spin Crossover Induced by Non-Covalent Interaction of a Metal–Organic Complex with N-Doped Graphene

Bruno Torre[1], Martin Švec [1], Rabindranath Lo[2], Debashree Manna[2], Amrit Sarmah[2], Dana Nachtigallová[2], Radek Zbořil[3], Pavel Hobza[2,3], Pavel Jelínek[1], Prokop Hapala[1]
[1]Institute of Physics of the Czech Academy of Sciences, Prague 6, Czech Republic. [2]Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Prague 6, Czech Republic. [3]Regional Centre of Advanced Technologies and Materials, Palacký University, Olomouc, Czech Republic

P079

The One-Electron Self-Interaction Error in 50 Density Functional Approximations

Dale Lonsdale, Lars Goerigk
The University of Melbourne, Melbourne, Australia

P080

The Effect of Ionic Liquids on the H_2 Splitting Capacity of Frustrated Lewis Pairs: Computational Insights

Kaycee Low[1], Lucy Brown[2], Małgorzata Swadźba-Kwaśny[2], Ekaterina Izgorodina[1]
[1]School of Chemistry, Monash University, Clayton, Australia. [2]The QUILL Research Centre, University of Belfast, Belfast, Ireland

P081

Effect of Factors on Ethylene Epoxidation by Oxoiron(IV) Porphyrin π-Cation Radical Complex in High Spin States: A DFT Study

Zhifeng Ma[1], Hiroshi Fujii[2], Masahiko Hada[1]
[1]Tokyo Metropolitan University, Tokyo, Japan. [2]Nara Women's University, Nara, Japan

P082

Determining the Mechanism of a Novel Class of Mitochondrial Uncoupler

Hugo MacDermott-Opeskin, Megan O'Mara
ANU, Canberra, Australia

P083

Theoretical Insights into CO_2 Hydrogenation to Methanol by a Mn–PNP Complex

Shyama Mandal[1], Kuber Rawat[1], Surajit Nandi[1], Biswarup Pathak[1,2]
[1]Discipline of Chemistry, Indian Institute of Technology Indore, Indore, India. [2]Discipline of Metallurgy Engineering and Materials Science, Indian Institute of Technology Indore, Indore, India

P084

Correlation Effects in the Photoelectron Spectrum and Photoionization Dynamics of OsO_4

Soumitra Manna, Sabyashachi Mishra
Indian Institute of Technology Kharagpur, Kharagpur, India

P085

Investigating the Effect of Protonation Site on Photostability

Samuel Marlton[1], Benjamin McKinnon[1], Boris Ucur[1], Stephen Blanksby[2], Adam Trevitt[1]
[1]UOW, Wollongong, Australia. [2]QUT, Queensland, Australia

P086

Polarisation of Water in Hydrated Choline Dihydrogen Phosphate and Related Ionic Liquids

Thomas Mason[1], Zoe Seeger[1], Anh Nguyen[1], Kyoko Fujita[2], Ekaterina Pas[1]
[1]Monash University, Melbourne, Australia. [2]Tokyo University of Pharmacy and Life Sciences, Tokyo, Japan

P087

MP2-Q-F12-SOS: A Novel Efficient Method to Compute the MP2-F12 Correlation Energy

Simon McKenzie, Peter Gill
University of Sydney, Sydney, Australia

P088

Photostability of Protonated Pyridine Derivatives in the Gas Phase

Benjamin McKinnon[1], Samuel Marlton[1], James Bezzina[1], Stephen Blanksby[2], Adam Trevitt[1]
[1]University of Wollongong, Wollongong, Australia. [2]Queensland Institute of Technology, Queensland, Australia

P089

Boron Nitride Nanotube Nucleation During Ni-Catalysed Chemical Vapour Deposition: Non-Equilibrium Molecular Dynamics

Ben McLean, Grant Webber, Alister Page
University of Newcastle, Callaghan, Australia

P090

A Mirror-Image Approach to Spin Contamination in Single-Determinant Wave Functions

Michael McTigue[1], Giuseppe Barca[1], Andrew Gilbert[1], Peter Gill[2]
[1]Australian National University, Canberra, Australia. [2]University of Sydney, Sydney, Australia

P091

Exploring the Applicability of Density Functional Approximations: The Most Comprehensive Benchmark Study of Double Hybrids and Application of Low-Cost DFT to Clam-Like Cyclotricatechylene Capsules

Nisha Mehta, Brendan Abrahams, Lars Goerigk
The University of Melbourne, Melbourne, Australia

P092

Full Atomistic Simulation of Ethylene/1-Octene Copolymerization Reaction Process Catalyzed by (Pyridylamido)Hf(IV) Complex

Nana Misawa[1], Yuichi Suzuki[1], Nobuaki Koga[1,2], Masataka Nagaoka[1,2,3,4]
[1]Nagoya University, Nagoya, Japan. [2]Future Value Creation Research Center, Nagoya University, Nagoya, Japan. [3]ESICB, Kyoto University, Kyoto, Japan. [4]JST-CREST, Tokyo, Japan

P093

Molecular Level Explanation of the Conversion of Regiospecificity (8R to 12S) in Lipoxygenase by a Single Mutation L434F

Vipin Mishra, Sabyashachi Mishra
Indian Institute of Technology, Kharagpur, India

P094

pH-Switchable Electrostatic Catalysis of Organo-SOMO Reactions

Ahmed Elaaf Mohamed, Michelle Coote
Australian National University, Canberra, Australia

P095

Theoretical Insights to Novel Beryllium Reactivity

Andrew Molino, David Wilson
La Trobe University, Melbourne, Australia

P096

Colloidal Stability of Apolar Nanoparticles

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A Computational Study of the Mechanism for the Enantiomerization of Tröger's Bases

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Molecular Dynamics Simulations on DNA Behaviour on Graphene Oxide and Reduced Graphene Oxide-PEG-NH2 in the Presence of Mg^{2+} and Cl^{-} ions

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Systematic Search for Crystal Structures of Dioxides of Group 14 Elements (CO_2, SiO_2, GeO_2) Under Ultrahigh Pressure

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Coordination Chemistry of Carbon

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Analytic First-Order Derivatives of Partially Contracted *N*-Electron Valence State Second-Order Perturbation Theory (PC-NEVPT2)

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Anion Dependences in Solution Structure and Ion Conduction Mechanism in Superconcentrated Electrolyte Solution for Na-Ion Batteries

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An AFIR Study on the Mechanism of the C-C Coupling Reaction of Borepin Derivatives via Oxidative Deborylation

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EPHI - An Embarrassingly Parallel Code for Calculating Molecular Hessians via PBS Queues

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Fergus Rogers, Michelle Coote
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Rationalising the Photochemistry of Atmospherically Important Carbonyls Through Theory and Structure

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Potential-Dependent Rates of Reaction for Hydrogen Evolution on MoS_2 Electrocatalysts

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Theoretical Study of Manganese Melilites and Related Structures

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Combining Modern Force Fields with ONIOM(QM:MM): The SICTWO Interface

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Anion Binding Affinity – Acidity versus Conformational Effects

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Semi-Local Machine-Learned Kinetic Energy Density Functional for Orbital-Free Density Functional Theory

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Theoretical Study on the Optical Properties of Multichromophoric Systems Based on an Exciton Analysis: Modification Guidelines

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Understanding the Mechanism of Oxidative Polymerisation of Phenols

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Machine Learning Protocol for Asymmetric Hydrogenation Catalysis

Sukriti Singh, Monika Pareek, Avtar Changotra, Sayan Banerjee, Bangaru Bhaskararao, Palaniappan Balamurugan, Raghavan Sunoj

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Microscopic Explanation of the Enantiomeric Excess in S_N1 Reaction in Solution: A Full Atomistic Simulation Study

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Computational Molecular Spectroscopy Leading the Way to New Physics

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Crystal Structure Prediction by Artificial Force Induced Reaction Method: Applications to Silicon Carbide

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Theoretical Study on the Reaction Mechanism of $Zn(OTf)_2$-Mediated Annulations of *N*-Propargylated Tetrahydrocarboline

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Large-Scale Quantum Mechanical Molecular Dynamics Simulations of Polaron Formation Process in a Lead Halide Perovskite Material Using Divide-and-Conquer Type Density-Functional Tight-Binding Method

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Cyclohexane Oxidation in Zeolites: Molecular Mechanism and Energetics

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Spectroscopic Investigation of 2-Phenylcyclobutanamine and Ethylbenzene Derivatives in the Gas-Phase

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Machine Learning for Predicting Electron Transfer Coupling in Organic Semiconductors

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Dominique Wappett, Lars Goerigk
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Directing the Self Assembly of Nanorods with Depletion Interactions

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Nitroxide Radical All-Organic Batteries in Ionic Liquid Electrolytes

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Methods to Improve the Calculations of SMD Solvation Free Energies and Associated pKa Values: Comparison between Choosing an Optimal Theoretical Level, Solute Cavity Scaling and Using Explicit Solvent Molecules

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Relativistic Effects in the K-Shell Photoionization Differential Cross Sections of Heavy Elements with the Complex Basis Function Method

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Competition Between Charge Migration and Charge Transfer Induced by Nuclear Motion Following Core Ionization: Model Systems and Application to Li_2^+

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Linear-Scaling Divide-and-Conquer Finite-Temperature Self-Consistent Field for Static Correlation Systems

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Re-Examination of Proline-Catalyzed Intermolecular Aldol Reaction: A Theoretical Study of the Mechanism and Stereoselectivity

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Mechanistic Investigation of the Intramolecular C–H Bond Silylation by Silacyclobutane

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Reaction Paths for Methacrolein with Low Energy Barriers

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Bimetallic Alloys for CVD growth of Graphene and Carbon Nanotubes

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