台灣理論計算分子科學學會會員大會

General Meeting of Taiwan Theoretical and Computational Molecular Sciences Association (T^2CoMSA)

暨

2018 年理論計算化學小組九月研討會

Theoretical and Computational Chemistry September Conference 2018

Program

September 4, 2018

Ta-Shue Chou Memorial Hall, Institute of Chemistry, Academia Sinica

中央研究院 化學研究所 周大紓講堂

09:30-09:50 Registration opens

09:50-10:00 General Meeting of T2CoMSA

Session I Chair：Kaito Takahashi

NO.01 10:00-10:15 **Cheng-chau Chiu** 邱政超 (Academia Sinica)
" A Computational Study on H_2 Absorption in a Porous Framework Structure … and the Uncertainty of its Results"

NO.02 10:15-10:30 **Abdul Hannan Khan** (National Taiwan University of Science and Technology)
" Computational Study of Methane Storage in Metal Organic Framework (MOF-74-Ni)"

Invite 10:30-10:50 **Dr. Yi-Cheng Cheng** 程一誠 所長
(Materials & Electro-Optics Research Division , National Chung-Shan Institue of Science and Technology 中山科學院 材料暨光電研究所)
"中科院與學界在材料與光電基礎領域的合作機會與挑戰"

10:50-11:05 Coffee Break

Session II Chair：Hsin-Tsung Chen / Shih-I Lu

NO.03 11:05-11:20 **Bing-Cheng Ji** 紀秉承 (National Taiwan University of Science and Technology)
" Theoretical Study of CO Oxidation on IrO_2(110) Surface"

NO.04 11:20-11:35 **Chen-Cheng Liao** 廖振成 (National Taiwan Normal University)
" Mechanistic Study of Hydrogen Evolution Reaction on Single Atomic Platinum Catalyst"

NO.05 11:35-11:50 **Chun-Chih Chang** 張鈞智 (National Taiwan Normal University)
" A Computational Exploration on CO Reduction via CO Dimerization on Mixed-Valence Copper Oxide Surface"

NO.06 11:50-12:05 **Yu-Te Chan** 詹侑得 (National Taiwan Normal University)
" Enhancing C-C Bond Formation by the Surface Strain: Investigating the C2 and C3 Intermediate Formation on the Grain Boundary Regions"

NO.07 12:05-12:20 **Ranganathan Krishnan** 任剛 (Chung Yuan Christian University)
" Theoretical Evidence of CO Oxidation on Pt Supported Penta-Graphene: A Density Functional Study"

12:20-13:30 Lunch break

13:30-14:30 Poster session

Session III Chair：Liang-Yan Hsu

NO.08 14:30-14:45 **Petra Shih** 施欣妤 (National Taiwan University)
" A Theoretical Study on the $Q_x \rightarrow Q_y$ Internal Conversion in Chlorophylls"

NO.09 14:45-15:00 **Jen-Hao Ou** 歐人豪 (National Taiwan University)
" Band Structure of the Incommensurate Quasi-One-Dimensional Chromium Extended Metal Atom Chain"

NO.10 15:00-15:15 **Wei-Chih Chen** 陳威智 (National Taiwan University)
" A Theoretical Study of Vibronic Coupling in Different Excited States of Polycyclic Aromatic Hydrocarbons"

Session IV Chair：Jen-Shiang Yu

NO.11 15:15-15:30 **Yun-Wen Chen** 陳韻文 (Academia Sinica)
" Wide Bandgap Tunability of Halide Perovskites via Volumetric Strain"

NO.12 15:30-15:45 **Wan-Yi Lin** 林宛儀 (National Taiwan University of Science and Technology)
" A DFT Study on Water Adsorption on Boron Doped Carbon Nanotubes: Effects of Doping Concentration"

NO.13 15:45-16:00 **Jheng-Hua Luo** 羅正華 (National Cheng-Kung University) [中文演講]
" Dual Functions of Water in Stabilizing the Metal-Pentazolate Hydrates $[M(N_5)_2(H_2O)_4]\cdot 4H_2O$ (M = Mn, Fe, Co, and Zn) High-Energy Density Materials"

16:00-16:15 Coffee Break

Session V Chair：Hsing-Yin Chen

NO.14 16:15-16:30 **Ming-Hsiu Hsieh** 謝明修 (National Chiao Tung University)
" Theoretical Investigation of Fragmentation Mechanisms of Thaimin in Transketolase – the Role of Glu418"

NO.15 16:30-16:45 **Zih-Jie Tai** 戴子傑 (National Taiwan University of Science and Technology)
" The First Principle Molecular Dynamic Simulation of the Electrolyte Reduction Mechanisms with/without Anode for Li-ion Battery"

Invite 16:45-17:05 校友經驗交流之一: 朱沛全 先生
Alumni Experience Sharing (I): Mr. Pei-Chuan Chu

Invite 17:05-17:25 校友經驗交流之二: 李昇叡 博士
Alumni Experience Sharing (II): Dr. Sheng-Jui Lee

17:25-17:40 Closing (Awards) Ceremony **Chair：Pei-Kun Yang**

Information of Poster Session

P01	Hsaio-Tien Pai 白孝天	A Computational Exploration on CO_2 Reduction via C_2 dimerization on Mixed-Valence Cu_2O Surface
P02	Cheng-Ting Yu 余承庭	CO_2 Capturing by Covalent Organic Frameworks: A Molecular Dynamic Study
P03	I-Huan Wu 吳宜洹	Extension of the Kinetic Energy Partition Method to Many-body Systems
P04	Yuan-Jia Fan 范原嘉	Wannier Excitons of Carbon Nanotubes with Helical Symmetry
P05	Nadaraj Sathishkumar 陳少定	Hydrogen Storage on Boron and Nitrogen Doped Penta-graphene Studied by DFT Calculations
P06	Min-Shao Ku 辜敏韶	Computational Electrochemical Reduction of CO on Cu(711) surface
P07	Zong-Rong Ye 葉宗融	The Fluorescence of Organic Compounds Analyze via Machine Learning
P08	Yung-Chi Ge 葛詠綺	Unveiling the Substrate Channeling Dynamics of Prostacyclin Synthases by Molecular Dynamics Simulation and Small-Angle X-ray Scattering
P09	Tsai-Jung Liu 劉采容	On the Ligand Conformation of Extended Metal Atom Chains (EMACs): from Planar to Helical and Hemihelical
P10	Hao-Rong Tsai 蔡皓融	Molecular Dynamics Simulations of Transport and Structural Properties of sCO_2 by Adaptive Force Matching Method