Program

Time

Program

9:20 - 9:40 AM

Registration opens

Session I

Energy-related Materials

Chair: Prof. Yi-Pei Li

9:40 - 9:55 AM

O01 鄭湘蓉 Hsiang-Jung Cheng

Theoretical Study on the Interaction of Water with $Li_{10}GeP_2S_{12}$ Solid Electrolyte: Effects of Selenium Doping on Chemical Stability

9:55 - 10:10 AM

O02 林冠宇 Kuan-Yu Lin

New Insights into the N-S Bond Formation of Sulfurized-Polyacrylonitrile Cathode Material for Li-S Batteries

10:10 - 10:25 AM

***O03* 陳琮叡 Tsung-Ruei Chen**

Theoretical Study on Surface Carbonization of Si (100) Surface Using Acetylene

10:25 - 10:40 AM

O04 王元瑜 Yuan-Yu Wang

First-Principles Molecular Dynamics Study of Anode-Free Lithium Metal Batteries: Effects of Zn Doping and Excess Electrons on Electrolyte Decomposition

10:40 - 10:55 AM

O05 陳威智 Wei-Chih Chen

A Molecular Design Approach for Organic Molecules with an Inverted/small Energy Gap between the Singlet and Triplet Excited States

10:55 -11:10 AM

Coffee break

Session II

Biological Systems

Chair: Prof. Min-Yeh Tsai

11:10 - 11:25 AM

O06 林尚緯 Shang-Wei Lin

Molecular Dynamics Simulations Combined with Small-Angle X-ray Scattering for Characterizing the Enzyme Dynamics of Cytochrome P450 Proteins

11:25 - 11:40 AM

O07 蘇冠璇 Kuan-Hsuan Su

Cytochrome P450 Substrate Channel Regulates Catalytic Reactions

11: 40 - 11:55 AM

O08 Erickson Fajiculay

Biostoch: A Software Package for Symbolic and Numeric Biological Simulation

11: 55 - 12:20 AM

General Meeting of Taiwan Theoretical and Computational Molecular Sciences Association (T2CoMSA)

12:20 - 01:40 PM

Lunch break

(1:10 - 1:40 PM T2CoMSA第三屆第一次理監事會議 IB-311會議室)

1:40 - 2:50 PM

Poster Session

(國網中心討論會：IB-113會議室)

Session III

Reactions and Mechanisms

Chair: Prof. Yi-Jung Tu

2:50 - 3:05 PM

O09 謝明修 Ming-Hsiu Hsieh

Non-Valence Correlation-Bound States of Breslow Intermediate

3: 05 - 3:20 PM

O10 黃海 Thi Hai Huynh

A Computational Approach to Understand the Dissociation Process in Mass Spectroscopy of Fructose

3:20 - 3:35 PM

O 11 賴厚任 Hou-Jen Lai

Catalytic Performance of Ir_4 Cluster Supported on Anatase TiO_2 (101) for Steam Methane Reforming – A First-Principles Study

3:35 - 3:50 PM

O12 林品君 Pin-Jun Lin

Theoretical Study of Methane Conversion on the Fe_3O_4 (311) Surface Using Fenton Reagent

3:50 - 4:10 PM

Coffee break

Session IV

Machine Learning

Chair: Prof. Yuan-Chung Cheng

4:10 - 4:25 PM

O13 王俊壹 Chun-I Wang

Machine Learning for Charge Transfer Coupling: A Framework for Artificial Neural Networks

4:25 - 4:40 PM

O14 許鼎威 Ting-Wei Hsu

An Improved Machine Learning Model for the Prediction of Heat of Formation

4:40 - 5:20 PM

Discussion

Chair: Prof. Yuan-Chung Cheng

Award Ceremony

Chair: Prof. Jyh-Chiang Jiang