

## PT-Physical and Theoretical Chemistry

**Friday, 26 January 2024, Room: Amber 4**

**Chair:** Kaito Takahashi, Institute of Atomic and Molecular Sciences, Academia Sinica

**Co-Chair:** Siriporn Jungsuttiwong, Ubon Ratchathani University

Time	Code	Title	Presenter
13.00 – 13.30	PT-I-01	Importance of noncovalent interactions in homogeneous and enzymatic catalysis	Seiji Mori
13.30 – 14.00	PT-I-02	Theoretical study on the role of dynamics during enzyme catalysis	Toshifumi Mori
14.00 – 14.15	PT-O-01	The development of a new hypothetical MOF database for high-efficiency MOFs targeted for CO <sub>2</sub> utilization	Poobodin Mano
14.15 – 14.30	PT-O-02	Computational investigation of double-atoms catalysts decorated on defective boron nitride for catalyzing CO oxidation: A DFT study	Ratchadaree Intayot
14.30 – 14.45	PT-O-03	Enhanced formic acid production through catalytic CO <sub>2</sub> hydrogenation on frustrated Lewis pair functionalized UiO-67	Pimjai Pimbaotham
14.45 – 15.00	PT-O-04	A DFT study on a single transition metal doped C <sub>3</sub> N for CO oxidation reaction	Suparada Kamchompoo
15.00 – 15.15	<b>Coffee Break</b>		
15.15 – 16.00	<b>PL-02 at Bhiraj Halls II and III</b>		



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**Friday, 26 January 2024, Room: Amber 4**

**Chair:** Seiji Mori, Ibaraki University

**Co-Chair:** Cheng-Chau Chiu, National Sun Yat-sen University

Time	Code	Title	Presenter
16.00 – 16.30	PT-I-05	A net zero climate-resilient future: A computational chemistry approach for energy solutions	Siriporn Jungsuttiwong
16.30 – 16.45	PT-O-05	The effect of non-metal doped graphitic carbon nitride for carbon dioxide reduction reaction: A DFT study	Wassana Mongkonkan
16.45 – 17.00	PT-O-06	Enhancing carbon dioxide reduction through single and dual heteroatoms doped diamond: A DFT study	Yuwanda Injongkol
17.00 – 17.15	PT-O-07	How many water molecules react with simplest Criegee intermediates at atmospheric conditions?	Kaito Takahashi
17.15 – 18.15	<b>Poster Session I at Bhiraj Hall 1</b>		
18.15 – 21.00	<b>Conference Banquet at Bhiraj Halls II and III</b>		

## PT-Physical and Theoretical Chemistry

**Saturday, 27 January 2024, Room: Amber 4**

**Chair:** Supawadee Namuangruk, Nanotec

**Co-Chair:** Luckhana Lawtrakul, Thammasart University

Time	Code	Title	Presenter
09.45 – 10.15	PT-I-04	Modeling the defective structure of MoS <sub>2</sub> : A first-principles kinetic Monte Carlo study	Cheng-chau Chiu
10.15 – 10.30	PT-O-08	Enhancing V <sub>2</sub> O <sub>5</sub> cathodes in magnesium-Ion batteries through aqueous electrolyte-induced hydrogen insertion: A first-principles approach	Suwit Suthirakun
10.30 – 10.45	PT-O-09	Roles of reactants for Suzuki C-C cross-coupling reaction using molecular volcano plots	Kwanchanok Kaewkwan
10.45 – 11.00	<i>Coffee Break</i>		
11.00 – 12.00	<i>Poster Session II at Bhiraj Hall I</i>		
12.00 – 13.00	<i>Lunch at EH100</i>		
<p><b>Chair:</b> Suwit Suthirakun, Suranaree University of Technology  <b>Co-Chair:</b> Prapasiri Pongprayoon, Kasetsart University</p>			
13.00 – 13.30	PT-I-03	Exploring human serum albumin modifications: Advancing screening and monitoring for non-communicable diseases	Deanpen Japrungr
13.30 – 13.45	PT-O-10	Molecular docking and dynamic simulations of anti-apoptotic Bcl-2 proteins as targets for bioactive compounds in <i>Durio zibethinus</i> for anti-cancer activity	Luckhana Lawtrakul