



## Physical Chemistry (PH)

**Session PH1**

**Room# BB 211**

**Date Feb 2, 2017**

**Time 14:30-16:00**

**Conductor:** Assoc. Prof. Dr. Vudhichai Parasuk

**Co-conductor:** Assoc. Prof. Dr. Siwaporn Meejoo Smith

Time	Code	Presenter	Title
14:30-15:00	PH-I-001	Prof. Dr. Durand Alain, Université de Lorraine, France	Adsorption of some biopolymers at interfaces for producing aqueous dispersions
15:00-15:15	PH-O-001	Kulpavee Jitapunkul, Thammasat University, Thailand	Molecular docking investigation on anti-asthmatic properties of natural compounds from Plai
15:15-15:30	PH-O-002	Ria Armunanto, Universitas Gadjah Mada, Indonesia	Structural and dynamical properties of myricetin tyrosine kinase complex in water: Molecular dynamics simulation study
15:30-15:45	PH-O-003	Wahyu Dita Saputri, Universitas Gadjah Mada, Indonesia	The solvation properties of Cu <sup>+</sup> in liquid ammonia: A quantum mechanical charge field (QMCF) molecular dynamics study
15:45-16:00	PH-O-004	Jitpinan Teanwarawat, Kasetsart University, Thailand	Electrochemical properties of Rhodamine B derivative: Experimental and DFT based approach

**Session PH2**

**Room# BB 211**

**Date Feb 2, 2017**

**Time 16:15-18:00**

**Conductor:** Prof. Dr. Durand Alain

**Co-conductor:** Assoc. Prof. Dr. Yuthana Tantirungrotechai

Time	Code	Presenter	Title
16:15-16:45	PH-I-002	Assoc. Prof. Dr. Deva Priyakumar Udayakumar, International Institute of Information Technology, India	Substrate adsorption on the catalytic and dynamic properties of metal nanoclusters
16:45-17:00	PH-O-005	Karan Bobuatong, Rajamangala University of Technology Thanyaburi, Thailand	Theoretical mechanistic investigation of Au <sub>8</sub> and Au <sub>6</sub> Pd <sub>2</sub> catalyzed aerobic oxidation of benzyl alcohol and ethanol to benzaldehyde and acetaldehyde
17:00-17:15	PH-O-006	Yutthana Wongnongwa, Ubon Ratchathani University, Thailand	Theoretical study on the catalytic reduction mechanism of NO by CO on Ag <sub>7</sub> Au <sub>6</sub> cluster
17:15-17:30	PH-O-007	Chirawat Chitpakdee, National Nanotechnology Center, Thailand	Effects of Brønsted acid on the selective catalytic reduction of NO with NH <sub>3</sub> on over Ru-doped ceria catalyst investigated by DFT method: Synergetic effect of Lewis acid and Brønsted acid sites



17:30-17:45	PH-O-008	Chompoonut Runnim, National Nanotechnology center, Thailand	Theoretical study of halogenated activated carbon for mercury oxidation
17:45-18:00	PH-O-009	Jittima Meeprasert, National Nanotechnology Center, Thailand	DFT study on the synergistic effect of Pt <sub>5</sub> /MoO <sub>3</sub> catalyst on the hydrodeoxygenation of dimethyl sulfoxide

**Session PH3**

**Room# BB 404**

**Date Feb 3, 2017**

**Time 10:30-12:15**

**Conductor:** Assoc. Prof. Dr. Deva Priyakumar Udayakumar

**Co-conductor:** Assoc. Prof. Dr. Siriporn Jungstittiwong

Time	Code	Presenter	Title
10:30-10:45	PH-O-010	Nuttapon Yodsin, Ubon Ratchathani University, Thailand	Effect of platinum decorated carbon nanocones on hydrogen storage reactions: Theoretical study
10:45-11:00	PH-O-011	Rattanawalee Rattanawan, Ubon Ratchathani University, Thailand	Computational investigation of porphyrin sensitizers with various donor and acceptor substituents for dye-sensitized solar cells
11:00-11:15	PH-O-012	Sarinya Hadsadee, Ubon Ratchathani University, Thailand	Theoretical investigations on the roles of the electron donor and $\pi$ -linker in perylene dyes for dye-sensitized solar cells
11:15-11:30	PH-O-013	Taveechai Wititsuwannakul, Mahidol University, Thailand	Mechanistic study of nickel 3-bis(adamantan-2- yl)imidazolin-2-ylidene catalyzed C-O bond hydrogenolysis of 2-methoxynaphthalene by a density functional theory
11:30-11:45	PH-O-014	Natee Sirisit, Hokkaido University, Japan	What is the origin for mechanochromism of Gold (I) complex (C <sub>6</sub> F <sub>5</sub> Au) <sub>2</sub> (m-1,4-Diisocyano benzene) – Direct evidence for the presence of Auophilic interaction
11:45-12:00	PH-O-015	Tanabat Mudchimo, Ubon Ratchathani University, Thailand	Theoretical study on carbon-doped boron nitride nanosheet as a metal-free catalyst for NO reduction reaction
12:00-12:15	PH-O-016	Herlina Rasyid, Universitas Gadjah Mada, Indonesia	Molecular docking analysis on epidermal growth factor receptor wild type (EGFR <sup>WT</sup> ) with quinazoline derivatives as tyrosine kinase inhibitor
12:15-12:30	PH-O-017	Kanokorn Sudto, Kasetsart University, Thailand	Target identification of hopeahainol C for antibacterial activity