Poster Session

Computational Physics, Computational Fluid Dynamics and Solid Mechanics (PFD)

Code	Presenter	Title
PFD-P-1	Lanchakorn Kittiratanawasin	Finite Volume Scheme with Weighted Average Flux for Wet and Dry Shallow Water Simulations
PFD-P-2	Chewa Thassana	Image Processing for Astronomical Objects
PFD-P-3	Nuttapong La-Ongtup	Atomistic Simulation of Structural Evolution at Long Time Scales: Diffusion in the FCC NiAl System
PFD-P-4	Sorasit Buapong	The Effects of Stone-Wales Defect on Quantum Capacitance in Carbon Nanotube
PFD-P-5	Wiraporn Maithong	Stellar Spectrum Analysis from eShel Spectroscope

Poster Session

Computational Chemistry (CHE)

Code	Presenter	Title
CHE-P-1	Narissa Kanlayakan	Effects of Different Proton Donor and Acceptor Groups on Excited-State Intramolecular Proton Transfers of Amino-type and Hydroxy-type Hydrogen-Bonding Molecules: Theoretical Insights
CHE-P-2	Jack D'Amelio	Structural Screening of Photoactive Covalent Organic Frameworks
CHE-P-3	Chanatkran Prommin	Theoretical Studies of Excited State Proton Transfer of 2-(2'-Hydroxyphenyl)benzimidazole, 2-Hydroxybenzaldehyde, 1-Hydroxy-2-acetonaphthone, and Their Derivatives
CHE-P-4	Suparada Kimchompoo	Theoretical Study of Different Donor-and Acceptor-Type Effect in Push−Pull Porphyrin Dyes for Dye-Sensitized Solar Cells
CHE-P-5	Ruangchai Tarsang	Theoretical Study on Effect of Auxiliary Acceptor in Novel D-p-π-π-A Featured Sensitizers for Dye-Sensitized Solar Cells
CHE-P-6	Chattarika Sukpattanacharoen	Theoretical Study on Electronic and Optical Properties of Polythiophene, Polyfuran, Polypyrrole and Their Derivatives as Light-Emitting Materials
CHE-P-7	Malinee Promkatkaew	Theoretical Study on the Structural and Spectroscopic Properties of Cyanine Dyes as Fluorescent Dyes for DNA Detection
CHE-P-8	Rusrina Salaeh	Time-Dependent Density Functional Theory (TDDFT) Investigation on Electronic and Photophysical Properties of Derivatives of 3-Hydroxyflavone
CHE-P-9	Worawaran Thongnuam	Aldol Condensation of Benzaldehyde and Acetophenone on Zirconium Based Metal-Organic Framework: A DFT Study
CHE-P-10	Sarinya Hussadee	Carbon-Doped Boron Nitride Nanosheet: An Efficient Metal-Free Catalyst for Catalytic Oxidation of Carbon Monoxide
CHE-P-11	Nattida Maeboonruan	Confinement Effect on the Adsorption of Glucose, Hydroxymethylfurfural and Levulinic Acid on H-Zeolites (H-ZSM5, H-MOR and H-BEA)
CHE-P-12	Rathawat Daengngern	Dynamics Simulations of ESIPT Reactions of 2,5-bis(2'-benzoxazolyl)hydroquinone
CHE-P-13	Yutthana Wongnongwa	Mechanistic Study of CO Oxidation by N_2O over Ag_7Au_6 Cluster Investigated by DFT Methods
CHE-P-14	Phornphimon Maitarad	Nitrous Oxide Decomposition with CO Reducing Agent over Oxotitanium Porphyrin: A Theoretical Study
CHE-P-15	Saowalak Phikulthai	The Catalytic Reaction of Ethanol to Ethylene : A DFT Study
CHE-P-16	Wasinee Panjan	The Conversion of Methane to Methanol over the [Cu-O-Cu]2+/ZSM-5 Zeolite : a Density Functional Theory Study
CHE-P-17	Chanchai Sattayanon	The Effect of Small Gas Detection on Metal-Embedded MoS_2: DFT Study
CHE-P-18	Chan Inntam	The Influence of Silver Cluster Size and Carbon Nanotubes on CO Adsorption: A DFT Study
CHE-P-19	Karan Bobuatong	Theoretical Mechanistic Investigation of Au_{20} and $Au_{16}Pd_4$ Catalyzed Aerobic Oxidation of Benzyl Alcohol to Benzaldehyde

Code	Presenter	Title
CHE-P-20	Tanabat Mudchimo	Theoretical Study on Carbon-Doped Boron Nitride Nanosheet as a Metal-Free Catalyst for NO Reduction Reaction
CHE-P-21	Suppasith Assawabenjang	Theoretical Study on Olefin Polymerization Catalyst: Half-Titanocenes Containing Aryloxo Ligands
CHE-P-22	Thantip Roongcharoen	Warped Nanographene $C_{80}H_{30}$ as a Promising Catalyst for Nitric Oxide Decomposition
CHE-P-23	Warin Jetsadawisut	Coarse-Grained Molecular Dynamics Simulation of CorA Magnesium Channel in a Nanodisc
CHE-P-24	Paptawan Suwanhom	Computational Docking Study of 4-Oxo-N-(2-(Piperidin- 1-Yl)Ethyl)-4H-Chromene-2-Carboxamide as Acetylcholinesterase and Butyrylcholinesterase Inhibitors
CHE-P-25	Panisak Boonamnaj	Dimer Structure Stabilization of H_v1 C-terminal Domain by Salt Bridge Movements
CHE-P-26	Wiparat Hotarat	Enhanced Stability of Inclusion Complexes of Alpha-Mangostin with Hydrophilic Beta-Cyclodextrin; A Molecular Dynamics Simulation Study
CHE-P-27	Channarong Khrutto	MD Simulation of M2 Proton Channel in Different Phospholipid Bilayer Models
CHE-P-28	Pattama Wapeesittipan	Millisecond Protein Dynamics Does Not Control Catalysis in Cyclophilin A – Evidence from Molecular Dynamics Simulations
CHE-P-29	Theerayut Khempach	Molecular Calculations on Host-Guest Inclusion Complexes of Natural Insecticides: Squamocin and Nicotine
CHE-P-30	Nattaya Mekjirawat	Molecular Docking Investigation of WR99210 Analogues as Novel *M.tuberculosis* DHFR Inhibitors
CHE-P-31	Naruedon Phusi	Structure Based Drug Design of 4-Aminoquinilone Derivatives in DNA Gyrase B Subunit for Anti-Tuberculosis Agents Using Molecular Dynamic Simulations
CHE-P-32	Triet Le Huynh Minh	A Data Mining Approach to Determine the Hindered Internal Rotational Frequency for Chemical Species

Poster Session

Computational Biology and Bioinformatics (BIO)

Code	Presenter	Title
BIO-P-1	Wanwisa Panman	Amylose Wrapping on Single-wall Carbon Nanotube by Computational Study
BIO-P-2	Panupong Mahalapbutr	Computer-Based Drug Screening of Mansonone G Analogs Against Human DNA Topoisomerase II ATPase Domain
BIO-P-3	Phakawat Chusuth	Dynamics Behaviors of Active and Inactive EGFR TK Domains with Erlotinib Bound
BIO-P-4	Sirilak Kongkaew	How a T-Cell Antigen Receptor Recognizes Self-Peptide Leading Autoimmune
BIO-P-5	Nitchakan Darai	In Silico Screening of Chalcones Against Epstein-Barr Nuclear Antigen 1 Protein
BIO-P-6	Kamonpan Sanachai	In Silico Screening of Targeted Proteins for Developing Anticancer Agents
BIO-P-7	Napat Kongtaworn	MD Simulations of Three Designed TSX Structures with 50% Galactose-Removal in Explicit Water Solvent
BIO-P-8	Chonnikan Hanpaibool	Molecular Dynamics Study on MCR-1 In Mono-Zinc and Di-Zinc Forms
BIO-P-9	Peerapong Wongpituk	Structural Dynamics and Binding Free Energy of Neral Cyclodextrins Inclusion Complexes: Molecular Dynamics Simulation
BIO-P-10	Bodee Nutho	Susceptibility of Potent Inhibitors Against NS2B/NS3 Serine Protease of Zika Virus: A Molecular Dynamics Study
BIO-P-11	Nattawat Tantijaratchai	Virtual Screening for Tripeptide Inhibitors in Nnrti Binding Pocket of HIV-1 Reverse Transcriptase

Poster Session

High Performance Computing, Cloud Computing, Computer Science and Engineering (CSE)

Code	Presenter	Title
CSE-P-1	Pairat Tulyaprawat	A Numerical Model for Optimizing a Magnetic Regenerator
CSE-P-2	Prasarnphun Saisin	Automatic Control for Water Droplet on Metal Surface