Date : 12 Feb 2026				
Session : Physical and Theoretical Chemistry				
Room : G6				
Time	**Presentation Code**	**Topic**	**Presenter**	**Section**
14.30-14.55	PT-K-01	MolGPT: Generative Models for Chemistry	Prof. Dr. Deva Priyakumar	**Oral 1 A** **Chairman :** Prof. Dr. Siriporn Jungsuttiwong **Co-Chair :** Assoc. Prof. Dr. Nawee Kungwan
14.55-15.15	PT-I-01	Integrative Discovery of EGFR and JAK Inhibitors: From Virtual Screening to Cancer Cell Apoptosis	Assoc. Prof. Dr. Thanyada Rungrotmongkol	
15.15-15.35	PT-I-02	FMO-guided drug discovery and design	Asst.Prof. Kowit Hengphasatporn	
15.35-15.50	PT-O-01	Explainable Artificial Intelligence (AI)-Based Prediction Models for Antiviral Small Molecules	Dr. Ittipat Meewan	
15.50-16.10	**Coffee Break**			
16.10-16.30	PT-I-03	Protein Aggregation Observed by Molecular Dynamics Simulation	Prof. Dr. Hisashi Okumura	**Oral 1B** **Chairman** : Assoc. Prof. Dr. Thanyada Rungrotmongkol **Co-Chair :** Asst.Prof. Kowit Hengphasatporn
16.30-16.50	PT-I-04	Employing phase transition behavior of polypeptides to control protein function by heat	Asst. Prof. Dr. Cong Vu	
16.50-17.10	PT-I-05	Integrating Machine Learning with DFT for Precise Prediction of ^{13}C and ^{1}H NMR Shifts of Flavonols	Assoc. Prof. Dr. Thishana Singh	
17.10-17.25	PT-O-03	From AlphaFold Modeling to Steered Molecular Dynamics and Umbrella Sampling: AI-Driven Exploration of Full-Length Amyloid-β Dimerization Energetics	Mrs. KAVITHA J	

Date : 13 Feb 2026				
Session : Physical and Theoretical Chemistry				
Room : G6				
Time	**Presentation Code**	**Topic**	**Presenter**	**Section**
08.30-08.55	PT-K-02	Ab-Initio Modeling of Photoluminescence	Prof. Dr. Daniel Escudero	**Oral 2** **Chairman :** Prof. Dr. Siriporn Jungsuttiwong **Co-Chair :** Assoc. Prof. Dr. Nawee Kungwan
08.55-09.15	PT-I-06	Machine learning potential based understanding of humidity-induced phase transition in CALF-20	Dr. Kaito Takahashi	

Date : 13 Feb 2026				
Session : Physical and Theoretical Chemistry				
Room : G6				
Time	**Presentation Code**	**Topic**	**Presenter**	**Section**
09.15-09.35	PT-I-07	FIREBALL2020 – A revitalized paradigm for DFT molecular dynamics in an AI world	Prof.Dr. James Lewis	
09.35-09.50	PT-O-05	Bridging Quantum Simulations into Molecular Predictions: Density Functional Theory (DFT) and Machine Learning-Based Analysis on Simple Volatile Polar Compounds	Marc Andrie M. Bermundo	
09.50-10.05	PT-O-06	Statistical Mechanics Study of Hydrated Reline Deep Eutectic Solvent	Mr. Witchapon pluekrungrot	
10.05-14.30	**Coffee Break**			
14.30-14.55	PT-CST Award-02	Unraveling H_2 Dissociation in CO_2 Hydrogenation on Frustrated Lewis Pair-Functionalized UiO–67: DFT and Nuclear Quantum Effects	Asst. Prof. Dr.Nuttapon Yodsin	**Oral 3** **Chairman :** Prof. Dr. Siriporn Jungsuttiwong **Co-Chair :** Assoc. Prof. Dr. Nawee Kungwan
14.55-15.10	PT-O-07	CO_2-Laser-Driven Ultrafast Synthesis of Trimetallic Ni-Co-Cu Borate Enabling High-Performance Nitrate Reduction Catalysis and Zinc-Nitrate Batteries	Ms. Pimjai Pimbaotham	
15.10-15.25	PT-O-08	MOFs as catalytic platforms: single-atom sites and mixed-metal nodes for CO_2 reaction mechanisms	Dr. Sarawoot Impeng	

Date : 13 Feb 2026				
Session : Physical and Theoretical Chemistry				
Room : G5				
Time	**Presentation Code**	**Topic**	**Presenter**	**Section**
08.30-08.50	PT-I-08	Sunlight-driven detoxification of organic dyes and antibiotics in water	Assoc.Prof.Dr. Suwat Nanan	**Oral 3** **Chairman :** Assoc. Prof. Dr. Nipaphat Charoenthai **Co-Chair :** Assoc. Prof. Dr. Wikorn Punyain
08.50-09.05	PT-O-09	Exploring the effect of different proton donors and substituents on the photophysical properties and ESIPT process in 3-Hydroxyflavone derivatives	Mr. Hamza Mumtaz	

Date : 13 Feb 2026				
Session : Physical and Theoretical Chemistry				
Room : G5				
Time	**Presentation Code**	**Topic**	**Presenter**	**Section**
09.05-09.20	PT-O-10	Electrocatalytic Hydrogen Production of 2D Truxene-based Conductive Metal–Organic Frameworks: DFT and ML Studies	Ms. Monruedee Meerawan	
09.20-09.35	PT-O-11	Reactive Molecular Dynamic Simulations of Lithium Metal-Liquid Electrolyte Interface of Li-S Battery	Mrs. Mirella Maahury	
09.35-09.50	PT-O-12	Revealing the influence of topology and Ce substitution on the electronic properties of Zr-porphyrin MOFs for CO_2 photoreduction	Ms. Parichat Chaunket	
09.50-10.05	PT-O-13	From Molecules to Reactors: Modeling the Hydrogenolysis of Polyolefins	Mr. Shivan Bissesar	
10.05-10.20	PT-O-14	Computational Investigation of Intermolecular Interactions in Room-Temperature Ionic Liquids for μSR Probing	Mr. Michael Armstrong	

Poster Presentation II : 13 Feb 2026		
Session : Physical and Theoretical Chemistry		
Presentation Code	**Topic**	**Presenter**
PT-P-01	Control of Exothermic Effects in Vat Photopolymerization using Thermally Conductive Nanoparticle-Doped Resins	Mr.Kittipan Suwannachot
PT-P-02	Sterically Induced Twisting in BODIPY Chromophores for Photophysical Modulation: Synthesis and Photophysical Investigation	Ms.Julalak Kwansod
PT-P-03	Mechanism of H_2 Evolution on g-C_3N_4/ZnO Photocatalyst: A Theoretical Study	Mr.Ananda Thongyu
PT-P-04	Complete degradation of organic pollutants in water by magnetically separable Fe_3O_4/CQDs-ZnO photocatalyst under sunlight irradiation	Mr.Sattra Nonthing
PT-P-05	Structure-based design of cycloartane secondary amines: identification of a promising Topoisomerase II lead candidate	Dr.Muhammad Niyomdecha
PT-P-06	DFT insights into CO_2 activation and reduction on defective UiO-66(Zr) MOF	Ms.Jirapat Santatiwongchai

Poster Presentation II : 13 Feb 2026		
Session : Physical and Theoretical Chemistry		
Presentation Code	**Topic**	**Presenter**
PT-P-07	Theoretical investigation of BF_2-formazanates in nanostructured environments for photodynamic therapy	Dr.Pannipa Panajapo
PT-P-09	Structure-based virtual screening and biological validation of natural products as potential *M. tuberculosis* InhA inhibitors	Ms.Thimpika Pornprom
PT-P-10	On-the-fly Dynamics Simulations of 1,8-Di(pyridinyl)carbazole as a Case Study of Accepting-site Competition in the Excited State	Assoc.Prof.Dr.Rathawat Daengngern
PT-P-11	Photophysics of Zn(II) Complexes for Enhanced Photodynamic Therapy: A Comprehensive Theoretical Study	Ms.Nutchaya Petchsook
PT-P-12	Predicting Protein–Ligand Binding Free Energies Using GFN2-xTB (ALPB): Accuracy, Benchmarking, and Applications	Ms.Watcharin Kumaeum
PT-P-13	Theoretical study on the effects of substituents on photophysical properties of single benzene fluorophores	Mr.Thanapat Charoenkitkaset
PT-P-14	BioGraphormer3D: A Hybrid 3D Graph and SMILES Learning Framework for HER2 Small-Molecule Bioactivity Prediction	Mr.Suebpong Pruttipattanapong
PT-P-15	A data-driven approach to modeling drug synergy and antagonism	Asst.Prof.Dr.Supanida Piyayotai
PT-P-16	*In silico* assessments of novel aminoguanidine analogues against BSA for glycation control	Ms.Richemae Grace R. Lebosada
PT-P-17	Mechanistic Insights and Predictive Modeling of Organophosphate Hydrolysis via DFT and SISSO Machine Learning	Ms.Araya Putthabal
PT-P-18	Mechanistic Insights and Descriptor Analysis of Glyphosate Adsorption on Metal–Organic Frameworks $M_3(BTC)_2$ from Density Functional Theory Calculations	Dr.Anawat Thivasasith
PT-P-19	Understanding Electrolyte Behaviour for Pre-Plasma Electrolysis Conditions via MD Simulation	Dr.Angkana Khuenpetch
PT-P-20	Computational screening of metal-substituted HKUST-1 catalysts for CO_2 hydrogenation to formic acid	Ms.Wachiraporn Rattana
PT-P-21	High-throughput screening of homonuclear dual metal atom embedded on C_2N monolayers for enhanced ammonia electrosynthesis	Ms.Sutheethida Kalapakdee
PT-P-22	Electrocatalytic urea synthesis from carbon dioxide reduction reaction (CO_2RR) and nitric oxide reduction reaction (NORR): A theoretical study	Mr.Nakharin Phonarwut

Poster Presentation II : 13 Feb 2026		
Session : Physical and Theoretical Chemistry		
Presentation Code	**Topic**	**Presenter**
PT-P-23	Theoretical study of pt-cluster-doped poly(carbazole-sulfone-TEG) for plastic-waste electroreforming into hydrogen and value-added products	Ms.Kewalin Prabwongsa
PT-P-24	A DFT study of hydrogen evolution reaction on B- and BO-doped graphene catalysts	Ms.Chonthicha Phimthong
PT-P-25	Glucose Isomerization to Fructose over Isolated Zn and Cu Sites on Dealuminated BEA Zeolite	Ms.Siriya Sukhonthachat
PT-P-26	DFT Mechanistic Study of Poly(ethylene terephthalate) Glycolysis Catalyzed by Tertiary Amines	Ms.Sataporn Aimduang
PT-P-27	Mechanistic Insights into the Photodecarbonylation of π-Extended Flavonol for PDT	Ms.Siramol Photiganit