Plenary Lecture

Date Aug 3, 2017 **Room# Auditorium 3rd floor**

Chair: Asst. Prof. Putchong Uthayopas

Time	Code	Presenter	Title
09:50-10:35	PL-1	*Ms. Denise Ruffner* IBM, USA	Utilizing IBM Power Systems to Optimize Genomic Applications Compute

Chair: Assoc. Prof. Siriporn Jungsuttiwong

Time	Code	Presenter	Title
13:00-13:45	PL-2	*Prof. Dr. Masahiro Ehara* Institute for Molecular Science, Japan	Structure and Catalytic Activity of Nanocluster Catalysts

Plenary Lecture

Date Aug 4, 2017 **Room# Auditorium 3rd floor**

Chair: Dr. Manaschai Kunaseth

Time	Code	Presenter	Title
09:00-09:45	PL-3	*Prof. Dr. Aiichiro Nakano* University of Southern California, USA	Extreme-scale Atomistic Simulations of Nanomaterials
09:45-10:30	PL-4	*Dr. Ito Chao* Academia Sinica, Taiwan	Chemistry and Our Common Future

Chair: Dr. Anchalee Junkaew

Time	Code	Presenter	Title
13:00-13:45	PL-5	*Prof. Dr. Sukit Limpijumnong* Suranaree University of Technology, Thailand	Designing a Massive Coil to Shield JUNO from the Earth's Magnetic Field

Aug 3, 2017
Computational Physics and Fluid Dynamics

Session PFD1 **Time 10:50-12:00** **Room# cc307**

Chair: Asst. Prof. Warasak Sukkabot

Time	Code	Presenter	Title
10:50-11:15	PFD-I-1	*Arthit Vongachariya* Siam Cement Chemicals, Thailand	Advanced Process Modelling: A Key to Accelerate Development of Petrochemical Products
11:15-11:40	PFD-I-2	*Somboon Otarawanna* MTEC, NSTDA, Thailand	Finite Element Analysis for Fatigue Life Prediction of Alloy Wheels under Radial Loading
11:40-12:00	PFD-O-1	*Krittidej Chanthawara* Ubon Ratchathani Rajabhat University, Thailand	A Variable Multiquadric Shape Parameter in the Dual Reciprocity Boundary Element Method for Convection-Diffusion Problems

Session PFD2 **Time 13:45-15:00** **Room# cc307**

Chair: Assoc. Prof. Anucha Yangthaisong

Time	Code	Presenter	Title
13:45-14:10	PFD-I-3	*Siegfried Fritzsche* University of Leipzig, Germany	The Role of Lattice Flexibility of ZIF - Materials Used for Gas Separation
14:10-14:35	PFD -I-4	*Sittipong Komin* Ubon Ratchathani University, Thailand	Variational Optimization of Capping Atom Potentials for QM/MM Method
14:35-14:55	PFD-O-2	*Churtpong Choodet* Khon Kaen University, Thailand	Insight into the Interaction of 8-oxo-dG and DNA Aptamer by Molecular Dynamics Simulation for the Application in Biosonsor

Session PFD3 **Time 15:15-16:45** **Room# cc307**

Chair: Assoc. Prof. Teparksorn Pengpan

Time	Code	Presenter	Title
15:15-15:40	PFD-I-5	*Jessada Chureemart* Mahasarakham University, Thailand	Hybrid Design for Advanced Magnetic Recording Media: Combining Exchange Coupled Composite Media with Coupled Granular Continuous Media
15:40-16:05	PFD-I-6	*Phanwadee Chureemart* Mahasarakham University, Thailand	Spin Transport in Read Elements via Spin Accumulation Model
16:05-16:25	PFD-O-3	*Noppamas Yolai* Khon Kaen University, Thailand	Effect of Size, Shape and Surface Charge on Cellular Uptake of Gold Nanoparticles
16:25-16:45	PFD-O-4	*Rutchapon Hunkao* Mahidol University, Thailand	Empirical Tight-Binding Calculation of Electronic Structure of Mn-Doped ZnS Nanocrystals

Aug 3, 2017
Computational Chemistry

Session CHE1 **Time 10:50-12:00** **Room# cc305**

Chair: Assoc. Prof. Akira Nakayama

Time	Code	Presenter	Title
10:50-11:15	CHE-I-1	*Tetsuya Taketsugu* Hokkaido University, Japan	Computational Approach to Design of Non-Platinum Catalyst for Oxygen Reduction Reaction: Boron Nitride with Gold
11:15-11:40	CHE-I-2	*Panida Surawatanawong* Mahidol University, Thailand	Mechanisms of C-O Bond Activation and Oxygen Activation: Density Functional Study
11:40-12:05	CHE-I-3	*Minh Tho Nguyen* KU Leuven, Belgium	Recent Advances in the Determination of Structure and Bonding of Elemental Clusters

Session CHE2 **Time 13:45-15:00** **Room# cc305**

Chair: Prof. Lam K. Huynh

Time	Code	Presenter	Title
13:45-14:10	CHE-I-4	*Jun-ya Hasegawa* Hokkaido University, Japan	Theoretical Study of Frustrated Lewis Pair for Activation of Stable Chemical Bonds
14:10-14:35	CHE-I-5	*Kaito Takahashi* Academia Sinica, Taiwan	Substitution Effect in the Reaction Rate of Criegee Intermediates with Water Vapor
14:35-14:55	CHE-O-1	*Suwit Suthirakun* Suranaree University of Technology, Thailand	First-Principles Study of Sn-Doped V_2O_5 as Cathode Material of Li-ion Batteries

Session CHE3 **Time 15:15-16:45** **Room# cc305**

Chair: Asst. Prof. Tim Kowalczyk

Time	Code	Presenter	Title
15:15-15:40	CHE-I-6	*Jyh-Chiang Jiang* National Taiwan University of Science and Technology, Taiwan	Theoretical Approaches for Improving Overall Performances of Dye-Sensitized Solar Cells
15:40-16:05	CHE-I-7	*Arkira Nakayama* Hokkaido University, Japan	Catalytic Reactions at the Liquid/Metal-Oxide Interface: Role of the Acid-Base Sites
16:05-16:25	CHE-O-2	*Yuwanda Injongkol* Kasetsart University, Thailand	Nitrous Oxide Decomposition over Cu-BTC Metal-Organic Frameworks: A DFT Study
16:25-16:45	CHE-O-3	*Panchanit Piyakeeratikul* Vidyasirimedhi Institute of Science and Technology, Thailand	Influence of Metal Species in Porphyrin-Base Metal-Organic Frameworks on Carbon Dioxide Capture

Aug 3, 2017
Computational Biology and Bioinformatics

Session BIO1 **Time 10:50-12:00** **Room# cc306**

Chair: Asst. Prof. Thanyada Rungrotmongkol

Time	Code	Presenter	Title
10:50-11:15	BIO-I-1	*Ras Pandey* The University of Southern Mississippi, USA	Self-Organizing Structures of Proteins by a Coarse-Grained Model
11:15-11:40	BIO-I-2	*Norio Yoshida* Kyushu University, Japan	p*K*a Prediction in Biological Systems Based on the Statistical Mechanics Theory of Liquids
11:40-12:00	BIO-O-1	*Sasiporn Rattanasupha* King Mongkut's University of Technology Thonburi, Thailand	Backward Bifurcation of SEIR Epidemic Model with Treatment Function

Session BIO2 **Time 13:45-15:00** **Room# cc306**

Chair: Prof. Jen-Shiang K. Yu

Time	Code	Presenter	Title
13:45-14:10	BIO-I-3	*Hisashi Okumura* Institute for Molecular Science, Japan	Simulational Studies of Aß Amyloid Fibrils by Equilibrium and Nonequilibrium Molecular Dynamics Method
14:10-14:35	BIO-I-4	*Kiattawee Choowongkomon* Kasetsart University, Thailand	Computer-aided Drug Discovery: From Small Compounds to Protein Inhibitors Against Tyrosine Kinase of EGFR
14:35-14:55	BIO-O-2	*Kanyani Sangpheak* Chulalongkorn University, Thailand	*In Vitro* and *In Silico* Studies of Chalcone as a New Anticancer Drug Candidate Against a Cancer Target Protein

Session BIO3 **Time 15:15-16:45** **Room# cc306**

Chair: Assoc. Prof. Vannajan Sanghiran Lee

Time	Code	Presenter	Title
15:15-15:40	BIO-I-5	*Jen-Shiang Yu* National Chiao Tung University, Taiwan	Enzyme Catalysis that Paves the Way for S-Sulfhydration *via* Sulfur Atom Transfer
15:40-16:05	BIO-I-6	*Satoru Itoh* Institute for Molecular Science, Japan	Oligomerization Pathway of Amyloid-Beta Fragments Studied by the Hamiltonian Replica-Permutation Method
16:05-16:25	BIO-O-3	*Suriyawut Kulatee* Thammasat University, Thailand	Enantioselectivity and Enzyme-Ligand Docking Studies of pfDHFR and Cycloguanil Compounds
16:25-16:45	BIO-O-4	*Kulpavee Jitapunkul* Thammasat University, Thailand	Molecular Modelling of 5-Lipoxygenase Enzyme with Antiasthmatic Substances from Plai

Aug 3, 2017

High Performance Computing, Cloud Computing, Computer Science and Engineering

Session CSE1 **Time 10:50-12:00** **Room# cc308**

Chair: Assoc. Prof. Vara Varavithya

Time	Code	Presenter	Title
10:50-11:15	CSE-I-1	*Zong-Yao Chen* ACER	AI in Practice: Application & Challenges
11:15-11:40	CSE-O-1	*Kunwithree Phramrung* King Mongkut's University of Technology Thonburi, Thailand	The Numerical Solution of Fractional Angiogenesis Problem by Meshless Local Petrov-Galerkin Method
11:40-12:00	CSE-O-2	*Naravadee Nualsaard* King Mongkut's University of Technology Thonburi, Thailand	The Meshless Local Petrov-Galerkin Method for Solving the New Black-Scholes-Schrodinger Model

Session CSE2 **Time 13:45-15:00** **Room# cc308**

Chair: Dr. Supakit Prueksaaroon

Time	Code	Presenter	Title
13:45-14:10	CSE-I-2	*Ekasit Kijsipongse* NECTEC, NSTDA, Thailand	Deep Learning on Hybrid GPU Cluster/Volunteer Computing
14:10-14:35	CSE-O-3	*Chanon Taupachit* Thammasat University, Thailand	Spinner: Failure Detection and Recovery Software in Software Define Network
14:35-14:55	CSE-O-4	*Soratouch Pornmaneerattanatri* Kasetsart University, Thailand	System Tuning for Energy Efficient Big Data Infrastructure

Session CSE3 **Time 15:15-16:45** **Room# cc308**

Chair: Dr. Chantana Chantrapornchai

Time	Code	Presenter	Title
15:15-15:40	CSE-I-3	*Waranyu Wongseree* King Mongkut University of Technology North Bangkok, Thailand	Climate Change Projections Using Statistical Downscaling
15:40-16:05	CSE-O-5	*Danupon Kumpanya* Rajamangala University of Technology Suvarnabhumi, Thailand	Application of Intensified Current Search to Design Optimal PIDD^2 Controller for BLDC Motor Speed Control with Back EMF Detection
16:05-16:25	CSE-O-6	*Peeranon Wattanapong* King Mongkut's University of Technology North Bangkok, Thailand	Express Lane Services on Software-Defined Networks
16:25-16:45	CSE-O-7	*Kanon Sujaree* Rajamangala University of technology Rattanakosin, Thailand	Blood Vehicle Routing Network Using Artificial Chemical Reaction Optimization Algorithm

Aug 4, 2017
Computational Physics and Fluid Dynamics

Session PFD4 **Time 10:45-12:00** **Room# cc307**

Chair: Dr. Sittipong Komin

Time	Code	Presenter	Title
10:45-11:10	PFD-I-7	*Norraphat Srimanobhas* Chulalongkorn University, Thailand	CMS Software and Computing: From RAW Data to Physics Results
11:10-11:35	PFD-I-8	*Teparksorn Pengpan* Prince of Songkla University, Thailand	Bloch Spectral Functions of Palladium-Doped Iron Telluride from KKR-CPA Calculations
11:35-11:55	PFD-O-5	*Umaporn Nuntaplook* Mahidol University, Thailand	The Scattering of Electromagnetic Waves from the Two-Layer Sphere When Outer Layer Has Variable Refractive Index: Shape Resonance

Session PFD5 **Time 13:50-15:00** **Room# cc307**

Chair: Asst. Prof. Jessada Chureemart

Time	Code	Presenter	Title
13:50-14:15	PFD-I-9	*Komsilp Kotmool* Mahidol Wittayanusorn School, Thailand	Predicting the High-Pressure Phases of Materials Using Evolutionary Algorithm
14:15-14:35	PFD-O-6	*Pakawat Toomjeen* Khon Kaen University, Thailand	Designing DNA-Functionalized AuNP Dimer by Molecular Dynamics Simulation for the Application in Biosensor
14:35-14:55	PFD-O-7	*Nissaya Chuathong* King Mongkut's University of Technology North Bangkok (Rayong Campus), Thailand	A New Hybrid Radial Basis Function: The First Step towards Numerically Solving Nonlinear PDEs

Session PFD6 **Time 15:15-16:45** **Room# cc307**

Chair: Asst. Prof. Phanwadee Chureemart

Time	Code	Presenter	Title
15:15-15:40	PFD-I-10	*Piti Ongmongkolkul* Mahidol University International College, Thailand	Current Computational Technique in High Energy Physics
15:40-16:00	PFD-O-8	*Warittha Thongkham* King Mongkut's University of Technology Thonburi, Thailand	Electrical Conductivity of Flexible PEDOT Thermoelectric Foams
16:00-16:20	PFD-O-9	*Witthawat Phanchai* Khon Kaen University, Thailand	Designing Colorimetric Aptasensor Based on Disassembly of AuNP Dimers for Detection of Ochratoxin A
16:20-16:40	PFD-O-10	*Nuttapon Yodsin* Ubon Ratchathani University, Thailand	Effect of Platinum Decorated Carbon Nanocones on Hydrogen Storage Reactions: Theoretical Study

Aug 4, 2017

Computational Chemistry

Session CHE4 **Time 10:45-12:00** **Room# cc305**

Chair: Dr. Kaito Takahashi

Time	Code	Presenter	Title
10:45-11:10	CHE-I-8	*Chao-Ping Hsu* Academia Sinica, Taiwan	Electronic Coupling and Rates for Singlet Fission
11:10-11:35	CHE-I-9	*Vinich Promarak* Vidyasirimedhi Institute of Science and Technology, Thailand	Functional Organic Materials for Optoelectronic Devices
11:35-11:55	CHE-O-4	*Suwapich Pornsatitworakul* Kasetsart University, Thailand	The Preparation of 5,7-Dihydroxy-4-Methylcoumarin via the Pechmann Reaction

Session CHE5 **Time 13:50-15:00** **Room# cc305**

Chair: Asst. Prof. Nawee Kungwan

Time	Code	Presenter	Title
13:50-14:15	CHE-I-10	*Lam K. Hunynh* Vietnam National University, Vietnam	Multi-Scale Modeling and Simulation for Gas-Phase Chemistry and Materials Design: Computational Tools and Applications
14:15-14:35	CHE-I-11	*Tim Kowalczyk* Western Washington University, USA	The Role of the Chemical Environment in Simulations of Photoactive Organic Materials
14:35-14:55	CHE-O-5	*Preeyaporn Poldorn* Ubon Ratchathani University, Thailand	A DFT Study of Volatile Organic Compounds Adsorption on Transition Metals Doped Single Vacancy Graphene

Session CHE6 **Time 15:15-16:45** **Room# cc305**

Chair: Asst.Prof. Panida Surawatanawong

Time	Code	Presenter	Title
15:15-15:40	CHE-I-12	*Min Gao* Hokkaido University, Japan	Reactivity of Gold Clusters in the Regime of Structural Fluxionality
15:40-16:05	CHE-I-13	*Manussada Ratanasak* Hokkaido University, Japan	Theoretical Study on Enantioselective Hydrosilylation of Styrene Catalyzed by Palladium with Helical Poly(quinoxaline-2,3-diyl)s Chiral Phosphine Ligand
16:05-16:25	CHE-O-6	*Kunanon Chattrairat* King Mongkut's Institute of Technology Ladkrabang, Thailand	A Theoretical Study of Small Schiff Base Complexes with Heavy Metal
16:25-16:45	CHE-O-7	*Supawadee Sainimnuan* Kasetsart University, Thailand	Binding Mode Study of Genistein in Complex with Estrogen Receptor Beta by Computational Methods

Aug 4, 2017
Computational Biology and Bioinformatics

Session BIO4 **Time 10:45-12:00** **Room# cc306**

Chair: Assoc. Prof. Kiattawee Choowongkomon

Time	Code	Presenter	Title
10:45-11:10	BIO-I-7	*Shinji Saito* Institute for Molecular Science, Japan	Reaction Model for Circadian Rhythm of Kai System Considering Elementary Processes
11:10-11:35	BIO-I-8	*Varomyalin Tipmanee* Prince of Songkla University, Thailand	Molecular Insight of Recombinant Interleukin-18 as a Model for Functional Protein Design
11:35-11:55	BIO-O-5	*Damrongrit Setsirichok* King Mongkut's University of Technology North Bangkok, Thailand	Effects of Incorporating Genetic Models into a Genetic Programming Tree Ensemble for Genetic Association Studies

Session BIO5 **Time 13:50-15:00** **Room# cc306**

Chair: Assoc. Prof. Norio Yoshida

Time	Code	Presenter	Title
13:50-14:15	BIO-I-9	*Peter Wolschann* University of Vienna, Austria	Databases in Chemistry and Biology
14:15-14:35	BIO-I-10	*Vannajan Sanghiran Lee* University of Malaya, Malaysia	Computational Design of Protein Inhibitor for Dengue Envelope Protein
14:35-14:55	BIO-O-6	*Damrongrit Setsirichok* King Mongkut's University of Technology North Bangkok, Thailand	Incorporating a Genetic Model into a Logistic Regression Model Improves SNP Selection by Lasso for Genetic Association Studies

Session BIO6 **Time 15:15-16:45** **Room# cc306**

Chair: Dr. Varomyalin Tipmanee

Time	Code	Presenter	Title
15:15-15:40	BIO-I-11	*Syed Sikander Azam* Quaid-i-Azam University, Pakistan	The Vitality of Swivel Domain Motion in Performance of Enzyme I of Phosphotransferase System; A Comprehensive Molecular Dynamics Study
15:40-16:05	BIO-I-12	*Sissades Tongsima* BIOTEC, NSTDA, Thailand	Sequencing Data Deluge: Thailand Challenges in Big Data Analytics
16:05-16:25	BIO-O-7	*Charis Georgiou* University of Edinburgh, United Kingdom	Pushing the Limits of Detection of Weak Binding Using Fragment Based Drug Discovery: Identification of New Cyclophilin Binders

Aug 4, 2017

High Performance Computing, Cloud Computing, Computer Science and Engineering

Session CSE4 **Time 10:45-12:00** **Room# cc308**

Chair: Dr. Waranyu Wongseree

Time	Code	Presenter	Title
10:45-11:10	CSE-I-4	*Chantana Chantrapornchai* Kasetsart University, Thailand	On the Fine Tuning CNN with Pretained Networks
11:10-11:30	CSE-O-8	*Krailerk Manopattanagorn* Kasetsart University, Thailand	The Development of a VM Auto-Scaling Software for OpenStack Cloud
11:30-11:50	CSE-O-9	*Kanon Sujaree* Rajamangala University of Technology Rattanakosin, Thailand	Mobile Dental Unit Using Computer Simulation Theory

Session CSE5 **Time 13:50-15:00** **Room# cc308**

Chair:

Time	Code	Presenter	Title
13:50-15:00			Special Session