DAILY PROGRAM

October 6, 2023 (Friday)

Registration and Welcome Reception	1F, Boya Lecture Building
Time	
16:00-18:00	Registration
18:00-20:00	**Welcome Reception**

October 7, 2023 (Saturday)

Rules for code: P = Plenary Speech; K = Keynote Speech; I = Invited Speech; O = Oral Presentation

Opening Ceremony	Room 101
Time	
08:45-09:00	**Opening Remarks**

Plenary Talk 1		Room 101
Chair: Jer-Lai Kuo, Academia Sinica		
Time	**Code**	
09:00-09:40	P1	**Ten Decades of Modeling Water** *Michael L. Klein, Temple University*
09:40-10:00	Group Photo and Coffee Break	

Session A-1 — 10:00-12:00 | Room 101

Chair: Chao-Ping Hsu, Academia Sinica

Time	Code	
10:00-10:30	KA 1-1	**Process Simulation by Machine Learning Potential** *Seungwu Han, Seoul National University*
10:30-10:50	IA 1-1	**Bond-Partitioning Energy Models and Their Applications** *Szu-Chia Chien, National Central University*
10:50-11:10	IA 1-2	**Inverse Design of Transition Metal Complexes with Desirable Spin States Using Deep Generative Models** *Tzu-Hsiung Nick Yang, National Tsing Hua University*
11:10-11:30	IA 1-3	**Advancing the Discovery of Next-Gen Antimicrobial Peptides Targeting WHO Top Pathogens: An Integration of Machine Learning Frameworks and Molecular Dynamics Simulations** *Hui-Hsu Gavin Tsai, National Central University*
11:30-11:45	OA 1-1	**Exploring the Mechanical Behavior of High Entropy Alloys with Exceptional Strength and Extensive Plasticity Through a Machine-Learned Potential Model** *Po-Yu Yang, Academia Sinica*
11:45-12:00	OA 1-2	**Computational Study of Collision-induced Dissociation of Sodiated Hex-HexNAc Disaccharides** *Hock-Seng Nguan, Academia Sinica*
12:00-13:00	Lunch	

Session A-2 — 10:00-12:00 | Room 102

Chair: Lee-Wei Yang, National Tsing Hua University

Time	Code	
10:00-10:30	KA 2-1	**Simulating Endosomal Escape of Lipid Nanoparticles** *Wataru Shinoda, Okayama University*
10:30-11:00	KA 2-2	**Vesicle Morphology Changes, Through Active Membrane Recycling** *Sunil Kumar, Indian Institute of Technology Madras*
11:00-11:20	IA 2-1	**Thermodynamic Parameters from Molecular Simulations: Insights into Lipid Nanodiscs and Sugar Glass** *Daniel Harries, The Hebrew University of Jerusalem*
11:20-11:40	IA 2-2	**Modulating the Phase Behaviors of Biomimetic Catanionic Bilayers** *Chi-Cheng Chiu, National Cheng Kung University*
11:40-12:00	IA 2-3	**Controlling Biological Membranes for Materials Applications** *Chang Yun Son, Pohang University of Science and Technology (POSTECH)*
12:00-13:00	Lunch	

Session A-3 — 10:00-12:00 | Room 103

Chair: Yuan-Chung Cheng, National Taiwan University

Time	Code	
10:00-10:30	KA 3-1	**Two-dimensional Vibrational Spectroscopy of Aqueous Solutions and Interfaces using a Combination of Simulations, Quantum Calculations and Machine Learning Methods** *Amalendu Chandra, Indian Institute of Technology Kanpur*
10:30-10:50	IA 3-1	**CAM-B3LYP Delivers Substantial Improvements to DFT and G_0W_0 Predictions of Bandgap and Spectroscopic Properties of Materials Compared to PBE, SCAN, HSE06, and PBE0** *Jeffrey Reimers, Shanghai University*
10:50-11:10	IA 3-2	**Investigate the Optical and Electronic of Organic NIR-II Fluorophores Dyes by the GW-BSE and TDDFT Approaches** *Nguyet N. T. Pham,* *University of Science, Vietnam National University Ho Chi Minh City*
11:10-11:25	OA 3-1	**Non-linear X-ray Adsorption Spectroscopy as a Probe of Buried and Functional Electrochemical Interfaces** *Tod A Pascal, University of California, San Diego*
11:25-11:40	OA 3-2	**Anharmonic Vibrational Analysis on the Near-Infrared Region of H_3O^+-X_n (X = Ar, N_2, and CO, n = 1-3)** *Qian-Rui Huang, Academia Sinica*
11:40-11:55	OA 3-3	**Optoelectronic and Charge Transfer Properties of Sumanene and its Heteroaromatic Analogues: A DFT Approach** *Chetti Prabhakar, National Institute of Technology Kurukshetra*
12:00-13:00	Lunch	

Session B-1 — 13:00-15:00 | Room 101

Chair: Ming-Kang (Brad) Tsai, National Taiwan Normal University

Time	Code	
13:00-13:30	KB 1-1	**Machine Learning for Fast Evaluation of Electron-Transfer Coupling** *Chao-Ping Hsu, Academia Sinica*
13:30-13:50	IB 1-1	**Structural Dynamics of Neighboring Water Molecules of N-Isopropylacrylamide Pentamer** *Gil C. Claudio, University of the Philippines Diliman*
13:50-14:10	IB 1-2	**Exploring Optimal Water Splitting Bifunctional Alloy Catalyst by Pareto Active Learning** *YongJoo Kim, Kookmin University*

14:10-14:30	IB 1-3	**Accelerated Neural Network Training through Dimensionality Reduction for High Throughput Screening of Quantum Materials** *Saswata Bhattacharya, Indian Institute of Technology Delhi*
14:30-14:45	OB 1-1	**Solvent Effects on *N*-Heterocyclic Carbene Formation in Ionic Liquids: A Reactive Molecular Dynamics Study** *John Paul Stoppelman, Georgia Institute of Technology*
14:45-15:00	OB 1-2	**A Neural Network Accelerated Search Scheme to Understand the Reactions of Di-saccharides** *Pei-Kang Tsou, Academia Sinica*
15:00-15:30	Coffee Break	

Session B-2

13:00-15:00 | Room 102

Chair: Ricky Bendanillo Nellas, University of the Philippines Diliman

Time	Code	
13:00-13:30	KB 2-1	**Systemic Feedback to Drug a Dancing Target on its Multiple Sites** *Lee-Wei Yang, National Tsing Hua University*
13:30-13:50	IB 2-1	**Extensive Sampling of Protein-Inhibitor Binding Landscapes using Molecular Dynamics Simulations** *Ai Shinobu, Osaka University*
13:50-14:10	IB 2-2	**Combining Molecular Dynamics Simulation and Machine Learning Based Analysis Methods, an Example of Monomer-Dimer Structures of SARS-Cov-2 Mpro Viral Protein** *Toan T. Nguyen, University of Science, Vietnam National University*
14:10-14:30	IB 2-3	**Molecular Dynamics Simulations of the Mechanism of Controlled Drug Release from Photoswitchable azo-PC Lipid Vesicles** *Steven Nielsen, The University of Texas at Dallas*
14:30-14:45	OB 2-1	**Molecular Modeling of Cannabis Compounds Blocking the Binding Between SARS-CoV-2 Spike Protein and Human Angiotensin-Converting Enzyme 2 Receptor** *Napat Kongtaworn, Chulalongkorn University*
14:45-15:00	OB 2-2	**The Crucial Role of the F-F' Loop in Inhibition of Cytochrome P450 3A: an in Silico Investigation** *Wan Wei, Agency for Science, Technology and Research (A*STAR)*
15:00-15:30	Coffee Break	

Session B-3 — 13:00-15:00 | Room 103

Chair: Sang Soo Han, Korea Institute of Science and Technology

Time	Code	
13:00-13:20	IB 3-1	**Initial Events in Photochemical CO_2 Reduction Reaction on 2D Transition Metal Dichalcogenides** *Michitoshi Hayashi, National Taiwan University*
13:20-13:40	IB 3-2	**Combined Density Functional Theory Calculation and Non-equilibrium Green's Function Approach to Predict the Sensitivity of Nitrogen-containing Gases over $PtTe_nS_{2-n}$ Monolayers (n =0 - 2)** *Chen-Hao Yeh, Feng Chia University*
13:40-13:55	OB 3-1	**Layer Distribution Study in 2D Perovskite Material using Machine Learning Enabled SNAP Potential and Hybrid Monte Carlo Method** *Svetozar Najman, Academia Sinica*
13:55-14:10	OB 3-2	**Description of Medium-Range Order in Amorphous Gese by Machine-Learned Potentials: Descriptor Versus Graph** *Minseok Moon, Seoul National University*
14:10-14:25	OB 3-3	**Excited-State Proton Transfer Reaction Catalyzed by Long-Range Hydrogen-Bond Relay** *Kuan-Hsuan Su, Fu Jen Catholic University*
15:00-15:30	Coffee Break	

Session C-2 — 15:30-17:30 | Room 102

Chair: Chi-Cheng Chiu, National Cheng Kung University

Time	Code	
15:30-16:00	KC 2-1	**Computer Simulation Methods for Long-Time and Large-Scale Biomolecular Transport** *Ioan Andricioaei, University of California Irvine*
16:00-16:20	IC 2-1	**Elucidating Protein-Ligand Binding Kinetics Based on Bimolecular Reaction Theory** *Kento Kasahara, Osaka University*
16:20-16:40	IC 2-2	**Biophysical Interpretation of Protein Engineering and Evolution by Molecular Modelling and Network Topology** *Thana Sutthibutpong, King Mongkut's University of Technology Thonburi*
16:40-17:00	IC 2-3	**Integrative Modeling of Biomolecular Dynamics from Molecular Dynamics Simulations and Single-Molecule Experiments** *Yasuhiro Matsunaga, Saitama University*
17:00-17:20	IC 2-4	**Impact of Proline Residues on the Oligomerization of Prion-like Polypeptides and their Effect on Amyloid Disruption** *Min-Yeh Tsai, National Chung Cheng University*
17:30-17:40	Break	

Session C-3 — 15:30-17:30 | Room 103

Chair: Hyungjun Kim, Korea Advanced Institute of Science and Technology

Time	Code	
15:30-15:50	IC 3-1	**New Methodology Combining Large-Scale Molecular Dynamics and Dynamic Monte Carlo Simulations to Study Gas Transport in Heterogeneous Media** *Tetsuro Nagai, Fukuoka University*
15:50-16:10	IC 3-2	**Benchmarking First-Principles Approaches for the Band Gap Prediction of Porous Materials** *Jung-Hoon Lee, Korea Institute of Science and Technology (KIST)*
16:10-16:30	IC 3-3	**Computational Study on the MOF/6FDA-DAM Interface in Mixed Matrix Membranes** *Bor Kae Chang, National Central University*
16:30-16:45	OC 3-1	**Machine Learning and Large-scale Molecular Simulations for Exploration of Metal-organic Frameworks in CO_2/CO Separation Application** *I-Ting Sung, National Taiwan University*
17:30-17:40	Break	

Plenary Talk 2 — Room 101

Chair: Jhih-Wei Chu, National Yang Ming Chiao Tung University

Time	Code	
17:40-18:20	P2	**Free Energetics of Solvation Analyzed through All-atom MD Simulation and a Density-functional Method** *Nobuyuki Matubayasi, Osaka University*

Poster Session and Dinner — 1F, Boya Lecture Building

Time	
15:00-17:40	Poster Setup
18:20-20:30	**Poster Session and Dinner**
20:30	Poster Removal

October 8, 2023 (Sunday)

Plenary Talk 3 — Room 101

Chair: Shiang-Tai Lin, National Taiwan University

Time	Code	
09:00-09:40	P3	**Atomistic Simulations of biochemical systems. The mechanism by which Agonists Activate G Protein-Coupled Receptors Complexed with G Protein; Basis for New Generations of Drugs with Maximum Activity and Minimized Side Effects** *William A. Goddard, California Institute of Technology*
09:40-10:00	Coffee Break	

Session D-1 — 10:00-12:00 | Room 101

Chair: Amalendu Chandra, Indian Institute of Technology Kanpur

Time	Code	
10:00-10:20	ID 1-1	**Supercooled Water in the Presence of Nanostructured Surface and Under Shear Flow** *Jayant K. Singh, Indian Institute of Technology Kanpur*
10:20-10:40	ID 1-2	**Non-Newtonian Rheology of Supercooled Liquids Near the Glass Transition** *Hideyuki Mizuno, The University of Tokyo*
10:40-11:00	ID 1-3	**Atomistic Simulations of Phase Transformation and Deformation Behaviors of Shape-Memory Alloys** *Won-Seok Ko, Inha University*
11:00-11:15	OD 1-1	**Analysis of Premelting Layers under Shear at Ice-Polymer Interface** *Takumi Sato, Keio University*
11:15-11:30	OD 1-2	**Large-Scale Molecular Dynamics Simulations for the Spreading Dynamics of Impinging Droplets on Solid Surfaces** *Takahiro Koishi, University of Fukui*
11:30-11:45	OD 1-3	**Molecular Simulation Methods for Tribology** *Hitoshi Washizu, University of Hyogo*
12:00-13:00	Lunch	

Session D-2

10:00-12:00 | Room 102

Chair: Daniel Harries, The Hebrew University of Jerusalem

Time	Code	
10:00-10:30	KD 2-1	**Conformational Dynamics and Association/Dissociation Processes of Biological Macromolecules Investigated by Advanced Molecular Simulation** *Akio Kitao, Tokyo Institute of Technology*
10:30-10:50	ID 2-1	**An Efficient Screening, an Accurate Evaluation, and a Simple Prediction of Protein Complex Structures** *Kazuhiro Takemura, National Tsing Hua University*
10:50-11:10	ID 2-2	**From the Single-Chain Behavior to Phase Behavior of Intrinsically Disordered Proteins** *Xiangze Zeng, Hong Kong Baptist University*
11:10-11:30	ID 2-3	**Molecular Simulation of Functional Motions in Biomolecular Machines** *Kei-ichi Okazaki, Institute for Molecular Science*
11:30-11:45	OD 2-1	**Bridging Atomic Details and Overall Kinetics: A Multiscale Computational Approach to Understand Peptide Self-Assembly** *Wei Han, Hong Kong Baptist University*
12:00-13:00	Lunch	

Session D-3

10:00-12:00 | Room 103

Chair: Chin-Hui Yu, National Tsing Hua University

Time	Code	
10:00-10:30	KD 3-1	**A New Dynamic Monte Carlo Method that can Generate Molecular Trajectories Statistically Satisfying Diffusion Equation with Position-Dependent Diffusion Coefficient and Potential** *Susumu Okazaki, The University of Tokyo*
10:30-10:50	ID 3-1	**Brownian Chain Molecular Dynamics: A Semiclassical Path Integral Approach** *Motoyuki Shiga, Japan Atomic Energy Agency*
10:50-11:10	ID 3-2	**A Molecular Theory of Crystal Nucleation from Dilute Phases** *Sudeep Punnathanam, Indian Institute of Science*
11:10-11:30	ID 3-3	**Topological Family Effect and Classification of Chiral Carbon Nanotubes *via* Natural Helical Symmetry** *Yu-Tzu Elise Li, National Taiwan Normal University*
11:30-11:45	OD 3-1	**Temperature Dependence of Energy Barrier in Kinetic Monte-Carlo Simulation using the Jarzynski Equality** *Atsushi M. Ito, National Institute for Fusion Science*
11:45-12:00	OD 3-2	**Developing a Model to Theoretically Assess the Turnover Frequency in the Light of Collision Theory** *Himangshu Pratim Bhattacharyya,* *Indian Institute of Technology Guwahati*
12:00-13:00	Lunch	

Session E-1 — 13:00-15:00 | Room 101

Chair: Jeffrey Reimers, Shanghai University and University of Technology Sydney

Time	Code	
13:00-13:20	IE 1-1	**Development and Applications of Reactive Force Fields of Carbon and Alloy** *Yi Liu, Shanghai University*
13:20-13:40	IE 1-2	**Effects of Electron-Phonon Interactions on the Electrical and Optical Properties of Semiconductors** *Youngho Kang, Incheon National University*
13:40-14:00	IE 1-3	**A Computational Approach for Predicting Dynamics and Structure of Organic Crystals** *Go Watanabe, Kitasato University*
14:00-14:20	IE 1-4	**Computational Design of Organic Materials in Optoelectronic Applications** *Kun-Han Lin, National Tsing Hua University*
14:20-14:35	OE 1-1	**Modeling the Charge and Exciton Transports in Organic Semiconductors** *Wei-Tao Peng, Academia Sinica*
14:35-14:50	OE 1-2	**Investigating Colossal Barocaloric Effect in Closo-type Hydrides using Molecular Dynamics Simulation** *Kartik Sau, Tohoku University*
15:00-15:30	Coffee Break	

Session E-2 — 13:00-15:00 | Room 102

Chair: Steven Nielsen, University of Texas at Dallas

Time	Code	
13:00-13:30	KE 2-1	**Early Stage Photodynamics of Photoactive Yellow Protein Simulated with the Interpolated Mechanics / Molecular Mechanics (IM/MM) Method** *Young Min Rhee,* *Korea Advanced Institute of Science and Technology (KAIST)*
13:30-13:50	IE 2-1	**Investigating Stability and Dynamics of Orexin 2 Receptor using Relaxation Mode Analysis and 3D-RISM Theory** *Ayori Mitsutake, Meiji University*
13:50-14:10	IE 2-2	**Enhanced Sampling using Machine Learning** *Bernd Ensing, University of Amsterdam*
14:10-14:30	IE 2-3	**Probing the Weak Interactions and Proton Transfer in Nanoscale Constraints** *Hsiao-Ching Yang, Fu Jen Catholic University*
14:30-14:50	IE 2-4	**Morphing Method Using the Trajectories of Molecular Dynamics Simulations and Deep Neural Network and the Applications** *Naoyuki Miyashita, KINDAI University*
15:00-15:30	Coffee Break	

Session E-3 — 13:00-15:00 | Room 103

Chair: Junming Ho, University of New South Wales (UNSW Sydney)

Time	Code	
13:00-13:20	IE 3-1	**DFT-CES: Eyes to See the Unseen, Buried Electric Double Layer** *Hyungjun Kim,* *Korea Advanced Institute of Science and Technology (KAIST)*
13:20-13:40	IE 3-2	**Atomistic Study on the Origins of the Anisotropic Lithiation Behaviors of the Silicon Anode Using the Reactive Force Field Based Molecular Dynamics Simulations** *Chin-Lung Kuo, National Taiwan University*
13:40-14:00	IE 3-3	**Weak Correlation between the Polyanion Environment and Ionic Conductivity in Amorphous Li–P–S Superionic Conductors** *Byungju Lee, Korea Institute of Science and Technology (KIST)*
14:00-14:20	IE 3-4	**Mechanistic Insight on Stability of Concentrated Electrolytes Near Lithium Metal Surface: Mechanism of Solid-Electrolyte Interphase (SEI) Formation** *Hemant Kumar Kashyap, Indian Institute of Technology Delhi*
14:20-14:40	IE 3-5	**Structure-capacitance Relationships for Nanostructured Carbon/Ionic Liquid Interfaces** *Yi-Jung Tu, National Chi Nan University*
14:40-14:55	OE 3-1	**First-Principles Methods for Halide Solid Electrolytes** *Chi-Hsuan Lee, Academia Sinica*
15:00-15:30	Coffee Break	

Session F-1 — 15:30-17:00 | Room 101

Chair: Nobuyuki Matubayasi, Osaka University

Time	Code	
15:30-16:00	KF 1-1	**Understanding the Anomalous Diffusion of Water in Aqueous Electrolytes using Machine Learning Potentials** *Balasubramanian Sundaram,* *Jawaharlal Nehru Centre for Advanced Scientific Research*
16:00-16:20	IF 1-1	**Explaining of Reaction Coordinates in Complex Molecular Systems Using Deep Learning and XAI: Application to Alanine Dipeptide Isomerization** *Kang Kim, Osaka University*
16:20-16:40	IF 1-2	**What do Deep Neural Networks Find in Disordered Structures of Glasses?** *Takeshi Kawasaki, Nagoya University*
16:40-17:00	IF 1-3	**Three Different Approaches to Extend Graph-Based Machine Learning for Molecular Property Prediction** *Hyun Woo Kim, Gwangju Institute of Science and Technology*
17:00-17:20	Break	

Session F-2 15:30-17:00 | Room 102

Chair: Lukman Hakim, Brawijaya University

Time	Code	
15:30-16:00	KF 2-1	**Molecular Simulation Studies on Soft Matter** *Bong June Sung, Sogang University*
16:00-16:20	IF 2-1	**Structure-Property Relationships on the Electrical Energy Loss of Polyimides through Molecular Simulation** *Tzu-Jen Lin, National Taiwan University of Science and Technology*
16:20-16:40	IF 2-2	**All-atom Molecular Dynamics Study of Fracture of Glassy Polymers** *Kazushi Fujimoto, Kansai University*
16:40-17:00	IF 2-3	**Rational Design of Amyloid Aggregation Inhibitors** *Jeong-Mo Choi, Pusan National University*
17:00-17:20	Break	

Session F-3 15:30-17:00 | Room 103

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

Time	Code	
15:30-15:50	IF 3-1	**Evolution Equations for the Short-Range Order Parameter: Application to Problems in Catalysis, Adsorption and Alloy Materials** *Abhijit Chatterjee, Indian Institute of Technology Bombay*
15:50-16:10	IF 3-2	**Important Role of CO_2 in C-N and C-C Bond Formation via Copper-Catalyzed Electrochemical Reduction** *Mu-Jeng Cheng, National Cheng Kung University*
16:10-16:30	IF 3-3	**A Computational Study of Phosphinous Acid-based Palladium Precatalysts in Hirao Cross-Coupling Reaction** *Wei-Chih Chen, Providence University*
16:30-16:45	OF 3-1	**Argentophilic Interactions, High Flexibility and Dynamic Properties of Pyrrole Cages Encapsulating Silver(I) Clusters** *Bartosz Trzaskowski, University of Warsaw*
17:00-17:20	Break	

Plenary Talk 4 — Room 101

Chair: Chun-Wei Pao, Academia Sinica

Time	Code	
17:20-18:00	P4	**The Molecular Ballet of Methane and Water to Form Gas Hydrates: Nucleation and Non-Vehicular Order Transmission** *David Tai-Wei Wu, Academia Sinica*

Banquet — LA MARÉE, Gongguan

Time	
18:30-20:30	**Banquet**

October 9, 2023 (Monday)

Plenary Talk 5 — Room 101

Chair: Li-Chiang Lin, National Taiwan University

Time	Code	
09:00-09:40	P5	**Big Data in Nanoporous Materials: Science beyond Understanding** *Berend Smit, Ecole Polytechnique Fédérale de Lausanne (EPFL)*
09:40-10:00	Coffee Break	

Session G-1 — 10:00-12:00 | Room 101

Chair: Padma Kumar Padmanabhan, Indian Institute of Technology Guwahati

Time	Code	
10:00-10:30	KG 1-1	**Multidimensional Free Energy Analysis of Electron and Ion Transfer Reactions Through Immiscible Liquid Interfaces** *Akihiro Morita, Tohoku University*
10:30-11:00	KG 1-2	**Acceleration and Analysis of Molecular Dynamics Simulations with Deep Learning Method** *Kenji Yasuoka, Keio University*
11:00-11:20	IG 1-1	**On the Correlated Motions of Ion Pairs in Ternary System of Ionic Liquids** *Lukman Hakim, Brawijaya University*
11:20-11:40	IG 1-2	**Hindered Diffusion near Fluid-Solid/Fluid Interfaces** *Ying-Lung Steve Tse, The Chinese University of Hong Kong*
11:40-11:55	OG 1-1	**Cosolvent Effects on Solvation and the Roles of Intermolecular-Interaction Components** *Stefan Hervø-Hansen, Osaka University*
12:00-13:00	Lunch	

Session G-2 — 10:00-12:00 | Room 102

Chair: Wataru Shinoda, Okayama University

Time	Code	
10:00-10:30	KG 2-1	**How Fast is Fast Enough: Computer Modeling of Host-guest Binding in a 3D Cell-adaptable Hydrogel Network** *Yi Wang, The Chinese University of Hong Kong*
10:30-11:00	KG 2-2	**Electrical Conductance of DNA/RNA: A Marker to Detect Intercalators, Oxidative Damage and Conformational Changes** *Prabal Kumar Maiti, Indian Institute of Science*

11:00-11:20	IG 2-1	**Phase Separation in a Binary Colloidal Mixture by Quorum Sensing Activity** *A. V. Anil Kumar, National Institute of Science Education and Research*
11:20-11:40	IG 2-2	**Computational Modeling of Polymer Membranes for Solvent Recovery** *Qisong Xu, Agency for Science, Technology and Research (A*STAR)*
11:40-12:00	IG 2-3	**On Structural and Transport Properties of Confined Water in Functional Soft Materials Investigated by Using All-Atom MD Calculation with Self-Consistent Modeling Scheme** *Yoshiki Ishii, Kitasato University*
12:00-13:00	Lunch	

Session G-3

10:00-12:00 | Room 103

Chair: Yi-Pei Li, National Taiwan University

Time	Code	
10:00-10:20	IG 3-1	**Activation of Hydrogen Peroxide by Cobalt(II) Hexaaqua and Cysteine Complexes: Classical Fenton-like and Nonclassical Mechanisms** *Hsing-Yin Chen, Kaohsiung Medical University*
10:20-10:40	IG 3-2	**PN^3(P)Pincer Complexes: Cooperative Catalysis and Beyond** *Kuo-Wei Huang,* *King Abdullah University of Science and Technology (KAUST)*
10:40-11:00	IG 3-3	**How Does Hydrogen Spillover Enhance the Activity for Ammonia Conversion? DFT Case Studies** *Hsin-Yi Tiffany Chen, National Tsing Hua University*
11:00-11:20	IG 3-4	**Theoretical Understanding of Oxygen Evolution Reaction on Nickel Oxyhydroxide Based Catalysts** *Hyeyoung Shin, Chungnam National University*
11:20-11:40	IG 3-5	**Electrochemical CO_2 Conversion into Platform Chemicals** *Supawadee Namuangruk,* *National Nanotechnology Center (NANOTEC)*
11:40-11:55	OG 3-1	**Exploration of B-doped Graphyne Family as Efficient Metal-Free Catalyst for C-C Coupling** *Klichchupong Dabsamut, Academia Sinica*
12:00-13:00	Lunch	

Session H-1

13:00-15:00 | Room 101

Chair: Susumu Okazaki, The University of Tokyo

Time	Code	
13:00-13:30	KH 1-1	**A Computational Molecular Technology for Complex Chemical Reaction Systems: Red Moon Approach** *Masataka Nagaoka, Nagoya University*
13:30-14:00	KH 1-2	**Atomistic Simulations: A Strong Driving Force Behind Research in Thermodynamics** *Jadran Vrabec, Technische Universität Berlin*
14:00-14:20	IH 1-1	**Effects of Chain Length on the Aggregate Structure of Perfluoroalkyl Oligomers** *Tomoko Mizuguchi, Kyoto Institute of Technology*
14:20-14:40	IH 1-2	**Investigating Cluster Structural Features from Homogeneous Nucleation of Binary Mixtures of Water, n-Nonane, 1-Butanol, and Ammonia using Molecular Dynamics** *Ricky Bendanillo Nellas, University of the Philippines Diliman*
14:40-14:55	OH 1-1	**Infrared Spectroscopy and Theoretical Structure Analyses of H^+(Methanol)m(Ethanol)n Clusters for m + n = 4** *Po-Jen Hsu, Academia Sinica*
15:00-15:20	Coffee Break	

Session H-2

13:00-15:00 | Room 102

Chair: Kaito Takahashi, Academia Sinica

Time	Code	
13:00-13:30	KH 2-1	**Graph-based Machine Learning Enabled Catalysts Design** *Sang Soo Han, Korea Institute of Science and Technology (KIST)*
13:30-13:50	IH 2-1	**Making Quantum Chemistry Compressive, Expressive and Parsimonious** *Jun Yang, The University of Hong Kong*
13:50-14:10	IH 2-2	**Strategies to Enhance the Accuracy and Efficiency of Computational Thermochemistry** *Junming Ho, University of New South Wales (UNSW Sydney)*
14:10-14:30	IH 2-3	**Quantum Electrodynamic Effects on Electron Transfer and Internal Conversion** *Liang-Yan Hsu, Academia Sinica*
15:00-15:20	Coffee Break	

Session H-3 — 13:00-15:00 | Room 103

Chair: Hemant Kashyap, Indian Institute of Technology Delhi

Time	Code	
13:00-13:30	KH 3-1	**Hybrid Machine Learning Energy Model for Discovery of High-Capacity Lithium Graphite Intercalation Phase** *Chun-Wei Pao, Academia Sinica*
13:30-13:50	IH 3-1	**Factors Governing Fast Ion Transport in Solids: Insights from Molecular Dynamics Simulations** *Padma Kumar Padmanabhan, Indian Institute of Technology Guwahati*
13:50-14:10	IH 3-2	**First-principles Study on the Stabilization of Oxidized Lattice Oxygen for High-Energy Li-Rich Cathodes** *Dong-Hwa Seo,* *Korea Advanced Institute of Science and Technology (KAIST)*
14:10-14:30	IH 3-3	**Simulation of Cathode Materials for Li- and Na-ion Batteries: from Electronic to Microscale** *Payam Kaghazchi, Forschungszentrum Jülich*
14:30-14:50	IH 3-4	**Towards Improved All-Solid-State Batteries: A Multi-Scale Simulation of Cation Interdiffusion and Mechanical Failures at NASICON-Oxide/$LiCoO_2$ Interfaces** *Hong-Kang Tian, National Cheng Kung University*
15:00-15:20	Coffee Break	

Plenary Talk 6 — Room 101

Chair: Michitoshi Hayashi, National Taiwan University

Time	Code	
15:20-16:00	P6	**Exploring Diffusion Behavior of Materials with Mobile Atoms using Machine-Learning Interatomic Potentials** *Ching-Ming Wei, Academia Sinica*

Closing Ceremony — Room 101

Time	
16:00-16:30	**Closing Remarks**