Program

21-Apr, Monday

Room 1

12:45-13:00 ***Opening***

Chair: Peter Gill

13:00-13:40 **1K1** **Shridhar Gadre**
Algorithm- and Code Development for ab initio studies on large molecules and Clusters

Chair: Satrajit Adhikari

14:00-14:25 **1A1** **Jinlong Yang**
Solving Many-Electron Schrodinger Equations with Artificial Intelligence

14:25-14:50 **1A2** **Lars Goerigk**
Insights into the one-electron self-interaction error in DFT

14:50-15:15 **1A3** **Debashree Ghosh**
Quantum chemistry methods to study strongly correlated systems – from variational to machine learning approaches

15:15-15:40 **1A4** **Bun Chan**
Data Quality in DFT Fitting

Chair: Cheol Ho Choi

16:00-16:25 **1A5** **Peifeng Su**
Theoretical methods for intermolecular interactions with qualitative and quantitative interpretations

16:25-16:50 **1A6** **Peter Gill**
A new approach to density functional quadrature

16:50-17:15 **1A7** **Eunji Sim**
Revisiting DC-DFT Error Decomposition and Its Extension: From Molecules to Solids

17:15-17:40 **1A8** **Minho Kim**
Efficient and Accurate van der Waals Correction for Density Functional Approaches in Material Simulations

Room 2

Chair: Jin Young Lee

14:00-14:25 **1B1** **Chang Woo Myung**
The Quest for Universal, Bayesian, and Equivariant Ab initio Machine Learning Potential: Bayesian Atoms Modeling (BAM) package

14:25-14:50 **1B2** **Rika Kobayashi**
The Landscape of Computational Chemistry in 2025

14:50-15:15 **1B3** **Hirotoshi Mori**
Electronic structure informatics for functional materials design: From methodology to experimental validation

15:15-15:40 **1B4** **Lin ji**
Coarse-grained dynamical state and nonequilibrium transition path analysis of combustion reaction system based on network community detection

Chair: Rika Kobayashi

16:00-16:25 **1B5** **Hao Dong**
High-precision molecular dynamics simulation methods accelerated by machine learning

16:25-16:50 **1B6** **Nguyen-Thi Van-Oanh**
Physcially Informed Machine Learning Potentials and Particle Swarm Optimization for Bimetallic Nanoparticles: Unlocking Structure-Property Insights

16:50-17:15 **1B7** **Junji Seino**
Systematic Accuracy Assessment of Quantum Chemical Calculations Using Machine Learning

17:15-17:40 **1B8** **Miho Hatanaka**
Preparation of a cerium complex dataset to evaluate the optical properties using machine learning

Room 3

Chair: Kai Chung Lau

14:00-14:25 **1C1** **Satoru Iuchi**
Molecular Dynamics Simulation to Understand Ultrafast Electronic Relaxation in Iron(II)-tris(bipyridine) Complex

14:25-14:50 **1C2** **Azusa Muraoka**
Modulating Charge Separation via Vibronic Coupling in Nonfullerene Organic Photovoltaics

14:50-15:15 **1C3** **Kumar Vanka**
Understanding the Behaviour of Unidirectional Molecular Motors with Computational Chemistry

15:15-15:40 **1C4** **Yuta Tsuji**
Exploration of the Origins of Quantum Interference

Chair: R.B. Sunoj

16:00-16:25 **1C5** **Junming Ho**
Fatty Alcohol Membrane Model for Quantifying Amphiphilicity

16:25-16:50 **1C6** **E. D. Jemmis**
An Extended Rudolph Diagram to explain the Structural Chemistry of Boron

16:50-17:15 **1C7** **Yu Harabuchi**
Exploring reaction and non-radiative decay paths using quantum chemical calculations: Reaction discovery through collaboration with experiments and informatics

17:15-17:40 **1C8** **Masahiro Ehara**
Photofunctional Metal Clusters and Heterogenous Catalysts: Collaborations with Experiment

Room 4

Chair: Ashwani kumar Twari

14:00-14:25 **1D1** **Jing Ma**
Prediction of NRR and CO2RR pathways and possible reaction intermediates

14:25-14:50 **1D2** **Haibo Yu**
Multiscale modelling to design potent inhibitors and high- performance biosensors

14:50-15:15 **1D3** **Phung Manh Quan**
Heterolytic vs. Homolytic Methane Hydroxylation: Insights from High-Level Theory

15:15-15:40 **1D4** **Mitsutaka Okumura**
Theoretical Study on TiOOH Production over Au Cluster Catalyst

Chair: Eluvathingal D. Jemmis

16:00-16:25 **1D5** **Elise Y. Li**
Electronic and Spintronic Innovations in Low-Dimensional Carbon Systems

16:25-16:50 **1D6** **Daisuke Yokogawa**
Development of solvation theory on the basis of Reference Interaction Site Model

16:50-17:15 **1D7** **Sang Uck Lee**
Machine Learning Potential assisted Energy Materials Research

17:15-17:40 **1D8** **Hirofumi Sato**
Theoretical Approaches to Chemical Phenomena in Condensed Phase

Reception Hall

13:40-14:00 ***Breaks***

15:40-16:00 ***Breaks***

18:00-20:00 ***Welcome Reception@Portopia Hotel***

22-Apr, Tuesday

Room 1

Chair: Jin Yong Lee

9:00-9:40 **2K1** **Hiromi Nakai**
Recent Advances of Electronic Structure Theory for Large Complex Systems

Chair: Lars Goerigk

9:55-10:20 **2A1** **Richard M.W. Wong**
Integrative AI-Driven Strategies for MDM2 Inhibitor Discovery Using Computational Techniques

10:20-10:45 **2A2** **Jer-Lai Kuo**
Connecting Potential Energy Surface with Experimental Observables with Human and Artificial Intelligence

10:45-11:10 **2A3** **Xiao Zheng**
Simulating Many-body Open Quantum Systems by Harnessing the Power of Artificial Intelligence and Quantum Computing

11:10-11:35 **2A4** **Biswarup Pathak**
Artificially Intelligent Nanopores for High-Throughput DNA Sequencing

11:35-12:00 **2A5** **Bo Thomsen**
Investigating Nuclear Quantum Effects in Supercritical Water

Chair: WanZhen Liang

14:00-14:40 **2K2** **Megan L O'Mara**
PolyConstruct: a generalized framework for MD simulations of complex biocompatible polymers

Chair: Haibo Ma

15:00-15:25 **2A6** **Ding Pan**
Development and Application of First-Principles Statistical Mechanics Methods for Studying Carbon-Bearing Supercritical Fluids

15:25-15:50 **2A7** **Hideaki Takahashi**
Density-Functional Theory Based on the Electron Distribution on the Energy Coordinate

15:50-16:15 **2A8** **Tim Gould**
Accurate ΔSCF from ensemble density functional theory

16:15-16:40 **2A9** **Amrit Sarmah**
Electrical Conductance Modulation in Peptides: Digital Decoding of Hydrogen-Bonding Patterns

16:40-17:05 **2A10** **Yingjin Ma**
Post-Density Matrix Renormalization Group (DMRG) implementations with and without reduced density matrices (RDMs)

17:05-17:30 **2A11** **Takeshi Iwasa**
Excited state engineering by photo-shaping using near-field

17:30-17:55 **2A12** **Sangita Sen**
Energy Response of Atomic and Molecular Orbitals in Non-uniform Magnetic Fields

Room 2

Chair: Hirotoshi Mori

9:55-10:20 **2B1** **Norio Yoshida**
Development of In-Silico Material Design Tool Based on the Molecular Theory of Solvation

10:20-10:45 **2B2** **Guiseppe Barca**
Exascale Ab Initio Molecular Dynamics with MP2 Accuracy

10:45-11:10 **2B3** **Henryk Witek**
Predicting stability of carbon nanostructures

11:10-11:35 **2B4** **Seunghoon Lee**
Simulating Ground-State Electronic Structure and X-ray Spectra of Transition-Metal-Sulfide Systems

11:35-12:00 **2B5** **Hong Jiang**
New developments in density-matrix based quantum embedding approaches to strongly correlated systems

Chair: Seung Kyu Min

15:25-15:50 **2B7** **Takashi Tsuchimochi**
Configuration interaction singles on top of configuration interaction singles

15:50-16:15 **2B8** **Jae Woo Park**
Multireference perturbation methods for exploring potential energy surfaces

16:15-16:40 **2B9** **Yoshio Nishimoto**
Analytic Derivatives of CASPT2 in OpenMolcas

16:40-17:05 **2B10** **Yang Guo**
Recent developments in multi-reference perturbation theory

17:05-17:30 **2B11** **Choi Cheol Ho**
MRSF-TDDFT: Expanding Application Scope of TDDFT

17:30-17:55 **2B12** **Hiroshi Nakatsuji**
Free Complement Theory combined with SAC/SAC-CI and Electrostatic Force Theories

Room 3

Chair: Min Gao

9:55-10:20 **2C1** **Hideo Ando**
Nuclear motion of Li+ under subnanoscale confinement in Li+@C60 salts

10:20-10:45 **2C2** **Kai Chung Lau**
Theoretical Insights into Structures and Energetics of Carbon Chains and Carbon Rings

10:45-11:10 **2C3** **Jin Wen**
Ultrafast Dynamics Simulations Accelerated by Machine Learning Models

11:10-11:35 **2C4** **Anoop Ayyappan**
Exploring Molecular Structures: Automation, ML Potentials, and Global Optimization

11:35-12:00 **2C5** **Manikandan Paranjothy**
Classical Trajectory Simulations of CN- + CH3I Bimolecular Nucleophilic Substitution Reaction

Chair: Toru Saito

15:00-15:25 **2C6** **Lung Wa CHUNG**
Reliable Protein-Drug Structures Enabled by Multi-scale and Machine Learning Methods

15:25-15:50 **2C7** **Jin Yong Lee**
Insight on the role of histidines in amyloid misfolding

15:50-16:15 **2C8** **Han Wei**
Multiscale Model for Computational Design of Peptide-Assembled Materials

16:15-16:40 **2C9** **Kazuhiro Fujimoto**
Spectral Tuning and Excitation-Energy Transfer in Photosynthetic Light-Harvesting Antennas

16:40-17:05 **2C10** **Thanyada Rungrotmongkol**
Targeting EGFR and JAKs for Cancer Therapy: In Silico Screening and Enhanced Anti-Cancer Efficacy

17:05-17:30 **2C11** **Xiang Sheng**
Computational Modeling and Rational Design of Enzymes

17:30-17:55 **2C12** **Shigehiko Hayashi**
Atomistically Deciphering Functional Activation Processes of Proteins with Hybrid Molecular Simulations

Room 4

Chair: Linjun Wang

9:55-10:20 **2D1** **Kazunari Yoshizawa**
Molecular Understanding of Adhesion from First-Principles Calculations

10:20-10:45 **2D2** **Bong June Sung**
A molecular simulation study on how entropy determines the mechanical properties of thermoplastic elastomers

10:45-11:10 **2D3** **Nicola Gaston**
Why is gallium liquid at room temperature?

11:10-11:35 **2D4** **Zhongyuan Lu**
Integrating Coarse-Grained Methods and Stochastic Reaction Models for Polymer Self-Assembly and Nanostructure Design

11:35-12:00 **2D5** **Akira Nakayama**
Molecular Insight into the Adsorption and Conversion at the Liquid/Solid-Oxide Interface

Chair: Wenjian Liu

15:00-15:25 **2D6** **Atsushi Ishikawa**
Multiscale Simulation from Density Functional Theory to Chemical Engineering Modeling

15:25-15:50 **2D7** **Bartosz Trzaskowski**
Fast tight-binding methods to study catalysts and mechanically interlocked systems

15:50-16:15 **2D8** **Jia-jia Zheng**
Mechanism-Guided Computational Screening of Nanomaterials for Medical Applications

16:15-16:40 **2D9** **Norifumi Yamamoto**
Simulating the Ancient Glow of Fireflies with Quantum Chemical Methods

16:40-17:05 **2D10** **Yuriko Aoki**
Linear scaling elongation method and its application to Bio-systems

17:05-17:30 **2D11** **Yasutaka Kitagawa**
Theoretical Study of Local Environmental Effects on Iron-Sulfur Clusters in Active Sites of Metalloproteins

Reception Hall

9:40-9:55 ***Breaks***

12:00-14:00 ***Poster&Lunch***

13:00-13:30 ***Fugaku tour@RIKEN R-CCS***

14:40-15:00 ***Breaks***

23-Apr, Wednesday

Room 1

Chair: Richard Ming Wah Wong

9:00-9:40 **3K1** **Donghui Zhang**
A quantitatively accurate universal potential for water

Chair: Hsiao Ching Yang

9:55-10:20 **3A1** **Tetsuya Taketsugu**
New Approaches to Understanding Chemical Reactions: Reaction Space Projector and Natural Reaction Orbitals

10:20-10:45 **3A2** **Liang-Yan Hsu**
Chemistry Meets Plasmon Polaritons and Cavity Photons: A Perspective from Macroscopic Quantum Electrodynamics

10:45-11:10 **3A3** **Ashwani kumar Twari**
Dynamics of Molecules under the Influence of Ultra Short Intense Laser Pulses

11:10-11:35 **3A4** **Chang Woo Kim**
Quantification of Dissipation Pathways in Chemical Quantum Dynamics

11:35-12:00 **3A5** **Jian Liu**
Nonadiabatic Field: A Conceptually New Approach for Nonadiabatic Transition Dynamics

Chair: Kimihiko Hirao

14:00-14:40 **3K2** **Francois Gygi**
From Pre-Exascale to Single-GPU: Implementation of the Qbox First-Principles Molecular Dynamics Code

Chair: Debashree Ghosh

15:00-15:25 **3A6** **Wei Li**
Recent Advances in the Cluster-in-Molecule Local Correlation Method for Large Systems

15:25-15:50 **3A7** **Hsiao Ching Yang**
From Proton Dynamics to Crystal Architecture: Multiscale Theory of Aqueous MOF Assembly

15:50-16:15 **3A8** **Seung Kyu Min**
Correlated Electron-Nuclear Dynamics for Extended Systems Based on Exact Factorization

16:15-16:40 **3A9** **Ha Quyen Nguyen**
Density Functional Methods For The Theoretical Modeling Of Auger Decay

16:40-17:05 **3A10** **Motoyuki Shiga**
Path Integral Brownian Chain Molecular Dynamics

17:05-17:30 **3A11** **WanZheng Liang**
Theoretical Modeling of Plasmon-Mediated Molecular Electronic Dynamics and Vibro-Polaritionic Spectra

17:30-17:55 **3A12** **Masanori Tachikawa**
Excess proton/deuteron in light/heavy water solvent using path integral molecular dynamics simulation

Room 2

Chair: Miho Hatanaka

9:55-10:20 **3B1** **William Dawson**
Reducing Numerical Precision Requirements in Quantum Chemistry Calculations

10:20-10:45 **3B2** **Yeonjoon Kim**
Leveraging Explainable Graph Attention Networks to Predict Vaporization Properties for Green Chemical Design

10:45-11:10 **3B3** **Jovan Jose K V**
New Developments and Applications of Graph Neural Network Approach for Accelerated Cluster Structure Prediction

11:10-11:35 **3B4** **Hyun Woo Kim**
Improving Mean-Field Ehrenfest Dynamics with Machine Learning for Two-State Model Simulations

11:35-12:00 **3B5** **Priyakumar Deva**
Machine Learning Algorithms for Self-Driving Chemistry Laboratories

Chair: Rahul Maitra

15:00-15:25 **3B6** **Lee-Wei Yang**
ADC-like Small Molecules Could Boost Clinical Success by Incorporating Systemic Feedback via MD Simulations and Generative AI

15:25-15:50 **3B7** **Chang Yun Son**
Modeling Classical and Quantum Charge Transport in Advanced Electronic Materials

15:50-16:15 **3B8** **Yuki Kurashige**
Tensor and Neural networks for quantum dynamics with many degrees-of-freedom

16:15-16:40 **3B9** **Jiajun Ren**
Quantum Dynamics Algorithms for Electron-Vibration Coupled Systems: Tensor Network and Quantum Computing

16:40-17:05 **3B10** **Taro Udagawa**
A Path Integral Molecular Dynamics Study on Proton-Bound Dimer Compound of Hydrogen Sulfate and Formate

17:05-17:30 **3B11** **Takao Tsuneda**
Reactive orbital energy theory: Theoretical foundations and applications

17:30-17:55 **3B12** **Zhendong Li**
Searching for Less Entangled Orbitals for Classical and Quantum Computing

Room 3

Chair: Anoop Ayyappan

9:55-10:20 **3C1** **Guixiang Zeng**
Theoretical Study on the Catalysis of Structural Constrained Phosphorus Compounds

10:20-10:45 **3C2** **Min Gao**
Factors Influencing Catalyst Activity: Insights from Computational Chemistry

10:45-11:10 **3C3** **Zhipeng Pei**
Unveiling the Diradical Nature of Quinodimethanes: Insights into Their Role in Organic Chemistry

11:10-11:35 **3C4** **Vudhichai Parasuk**
Exploring of Post/Non-Metallocene Catalysts for Ethylene Polymerization by Density Functional Theory

11:35-12:00 **3C5** **Jun-ya Hasegawa**
Reaction Mechanism and Catalyst Design of Transition Metal Complexes

Chair: Patchareenart Saparpakorn

15:00-15:25 **3C6** **Min-Yeh Tsai**
Through the Digital Microscope: Molecular Dynamics of Abeta Aggregation in Neurodegeneration

15:25-15:50 **3C7** **Toru Saito**
Molecular Simulation and Chemoinformatics studies on Inhibition Mechanism of Metalloenzymes

15:50-16:15 **3C8** **Yiqin Gao**
Modeling of biomolecules with the help of AI

16:15-16:40 **3C9** **Kiyoshi Yagi**
Development of QM/MM Methods in GENESIS and Applications to Biomolecular Reactions and Spectroscopy

16:40-17:05 **3C10** **Jun Soo Kim**
Pattern Formation on Phase-separating Lipid Vesicles by Uniaxial Compression

17:05-17:30 **3C11** **Zexing Cao**
QM/MM Insight into Enzymatic Oxidative Ring-Cleavage and Distant C-H Bond Activation by Fe(II) Dependent Oxygenases

17:30-17:55 **3C12** **Pradipta Bandyopadhyay**
Using a perturbation approach to optimize the scaling of charges in charge-scaling classical molecular dynamics simulations: Application to Protein loops

Room 4

Chair: Shigeyoshi Sakaki

9:55-10:20 **3D1** **Linjun Wang**
Detailed Complementary Consistency

10:20-10:45 **3D2** **Alessandro Pecchia**
Optical and transport properties of MoS2/WS2 bilayers with S-vacancies

10:45-11:10 **3D3** **Yusuke Ootani**
Molecular Dynamics Simulation Study on Mechanochemical Dynamics in Materials

11:10-11:35 **3D4** **Vikas Kashid**
Study of Magnetic Ground States in Compounds Involving Interactions Between 4f and 3d Electrons

11:35-12:00 **3D5** **Akihiro Morita**
Recent Development of Theoretical Analysis of Sum Frequency Generation Spectroscopy

Chair: Eunji Sim

15:00-15:25 **3D6** **Joonsuk Huh**
Quantum simulators for the multistate linear vibronic coupling model with Uracil cation

15:25-15:50 **3D7** **Yingzhou Li**
Quantum Orbital Minimization Method and Optimal Orbital Selection for Excited States Calculation

15:50-16:15 **3D8** **Atul Kumar**
Addressing Entanglement versus Separability Paradigm using Quantum Neural Networks

16:15-16:40 **3D9** **Takeshi Sato**
Quantum/classical hybrid simulations of intense laser-driven multielectron dynamics

16:40-17:05 **3D10** **Zhenyu Li**
Quantum Algorithms for Electronic Structure Problems

17:05-17:30 **3D11** **Soichi Shirai**
Analysis of chemical reactions by quantum chemical calculations using the quantum-classical hybrid algorithm

Reception Hall

9:40-9:55 ***Breaks***

12:00-14:00 ***Poster&Lunch***

13:00-13:30 ***Fugaku tour@RIKEN R-CCS***

14:40-15:00 ***Breaks***

24-Apr, Thursday

Room 1

Chair: Hiroshi Nakatsuji

9:00-9:40 **4K1** **Haibo Ma**
New quantum chemical approaches based on renormalized modes/states for large strongly correlated systems

Chair: Minh Tho Nguyen

9:55-10:20 **4A1** **Takuro Tsutsumi**
Visualization of Reduced-dimensional Potential Energy Surface by Reaction Space Projector (ReSPer)

10:20-10:45 **4A2** **Won June Kim**
First-principles studies on tuning the magnetization/polarization switching of the ferroic materials

10:45-11:10 **4A3** **Bin Jiang**
Full-dimensional First-principles Nonadiabatic Dynamics of Energy Transfer upon Molecular Collisions on Surfaces

11:10-11:35 **4A4** **Satrajit Adhikari**
Role of Electron-Nuclear Coupling: Spectroscopy, Scattering and Phase Transition

11:35-12:00 **4A5** **Kazuo Takatsuka**
Real-valued Schrodinger equation derived from scratch and single-event quantum-path dynamics: Celebrating 100 years of quantum mechanics

Room 2

Chair: Phung Thi Viet Bac

9:55-10:20 **4B1** **Rahul Maitra**
Resource Efficient Approach toward Dynamic Quantum Algorithms via Non-iterative Auxiliary Subspace Corrections

10:20-10:45 **4B2** **Jie Liu**
Hybrid Quantum-Classical Algorithms for Quantum Chemistry

10:45-11:10 **4B3** **Ray Miyazaki**
Materials Genes of CO2 Hydrogenation on Supported Cobalt Catalysts: an AI Approach Integrating Theoretical and Experimental Data

11:10-11:35 **4B4** **Chao-pin Hsu**
Machine Learned off-diagonal dynamics in charge transport

11:35-12:00 **4B5** **Jongkwon Ha**
Analog Quantum Simulation of Coupled Electron-Nuclear Dynamics in the Pre-Born-Oppenheimer Framework

Room 3

Chair: Phung Quan

9:55-10:20 **4C1** **Minh Tho Nguyen**
Aromaticity of Atomic Clusters: Electron Count Models Based on Geometrical Motifs

10:20-10:45 **4C2** **Shohei Yamazaki**
Photoreactions toward Conical Intersections in Indigo Isomers

10:45-11:10 **4C3** **Hiroki Uratani**
Origin of blue-shifted phosphorescence from an Ir(III) complex induced by encapsulation within a hydrogen-bonded organic cage

11:10-11:35 **4C4** **Takeshi Yoshikawa**
Kinetic analysis of domino-type dehydration-cyclization reaction of alkynols based on quantum chemical calculations

11:35-12:00 **4C5** **Shigeyoshi Sakaki**
Theoretical Study of Pd13 Cluster Complexes: Ligand Control of Cuboctahedral, Anticuboctahedral, and Icosahedral Structures

Room 4

Chair: Koichi Yamashita

9:55-10:20 **4D1** **Nahoko Kuroki**
Effective fragment potential molecular dynamics simulation for evaluating the hydration structures of amphiphilic molecules

10:20-10:45 **4D2** **Manyi Yang**
Influence of Surface Dynamics on Ammonia Catalytic Decomposition Process

10:45-11:10 **4D3** **Tuan Anh Pham**
Elucidating Structural Heterogeneity of Materials with Spectroscopy, Machine Learning, and Atomistic Simulations

11:10-11:35 **4D4** **Masahiro Higashi**
Theoretical Analysis of Excited State Properties in Solution and Protein

11:35-12:00 **4D5** **Shinji Saito**
Unveiling the Role of Dynamic Disorder in the Slowing Down of Supercooled Water Dynamics

Reception Hall

9:40-9:55 ***Breaks***

12:30-18:00 ***Excursion by own expense***

18:00-20:00 ***Banquet (Cruising)***

25-Apr, Friday

Room 1

Chair: Shridhar Gadre

9:00-9:40 **5K1** **Hyungjun Kim**
Development of Mean-field QM/MM to Elucidate Phase Transitions in Electric Double Layer Structure and Capacitance Peaks

Chair: Liang-Yan Hsu

9:55-10:20 **5A1** **Xiao He**
Recent Developments in the Quantum Fragmentation Methodology for Studying Large Molecules and Condensed-phase Systems

10:20-10:45 **5A2** **Luigi Genovese**
Flexibilities of wavelets as a computational basis set for large-scale electronic structure calculations

10:45-11:10 **5A3** **Masato Kobayashi**
Linear-scaling divide-and-conquer electronic structure methods for strongly correlated systems

11:10-11:35 **5A4** **Enhua Xu**
Distributed Implementation of Tensor-Product Bitstring Selected Configuration Interaction

Chair: Sangita Sen

14:00-14:25 **5A6** **Vikram Gavini**
Towards Large-scale Quantum Accuracy Materials Simulations

14:25-14:50 **5A7** **Marco Govoni**
Point Defects in Semiconductors Investigated with Time-Dependent Density Functional Theory, Many-body Perturbation Theory, and Quantum Embedding Methods

14:50-15:15 **5A8** **Siriporn Jungsuttiwong**
Advancing Battery Technologies for Renewable Energy Integration: Experimental and DFT Investigation

15:15-15:40 **5A9** **Abhilash Chandra**
Behavior of Water at Lipid/Water Interfaces upon Phase Transition of the Lipid Bilayer: Insights from 1D- and 2D-Vibrational Sum Frequency Generation Spectral Calculations from Molecular Dynamics Simulations

15:40-16:05 **5A10** **Takafumi Shiraogawa**
Antisymmetry Rules for Relationships of Material Properties in Chemical Compound Space

16:05-16:30 **5A11** **Yi Zhao**
Charge/Energy Transfer Dynamics in Extended Systems Simulated from Stochastic Schrodinger Equations

16:30-16:55 **5A12** **Ryohei Kishi**
Theoretical study on singlet fission dynamics in symmetric linear heterotrimer models

Chair: Nguyen-Thi Van-Oanh

17:15-17:55 **5K2** **Sonia Coriani**
Modeling Light-Matter Interactions and Spectroscopic Observables on Classic and Hybrid-Quantum Computers

17:55-18:20 ***Poster awards ceremony***
Closing

Room 2

Chair: Takao Tsuneda

9:55-10:20 **5B1** **Chen Li**
Novel method for solving Schrodinger equations and the Exact Analytic structure of many-body wave functions

10:20-10:45 **5B2** **Hiroyuki Nakashima**
Interstellar molecular chemistry with Schrodinger-level accuracy realized by the free complement theory

10:45-11:10 **5B3** **Jun-Ho Choi**
Molecular aggregation and microheterogeneity in various aqueous solutions

11:10-11:35 **5B4** **Ranajit Saha**
Unveiling Fluxional Dynamics in Calix[3]pyrrole: NMR Spectral Effects and Halide-Induced Conformational Control

11:35-12:00 **5B5** **Kimihiko Hirao**
Theoretical study of core electron binding energies for the third-period elements

Chair: Hiroyuki Nakashima

14:00-14:25 **5B6** **Chinami Takashima**
Development of Accurate and Efficient Relativistic Methods Based on Spin-free Infinite-order Two-Component Hamiltonian

14:25-14:50 **5B7** **Wenjian Liu**
Unified Implementations of Relativistic Hamiltonians and Wavefunctions

14:50-15:15 **5B8** **Subodh S. Khire**
Development of fragment-based algorithms for Advancing Quantum Chemical Investigations of Molecular Clusters

15:15-15:40 **5B9** **Priya**
A Green's function formalism for kinetic energy density functional in Orbital-free DFT

15:40-16:05 **5B10** **Jeheon Woo**
Efficient Density Functional Calculations on GPUs via Mixed Precision Approach

16:05-16:30 **5B11** **Shuhua Li**
Advances in Linear Scaling Local Correlation Methods

Room 3

Chair: Mitsuo Shoji

9:55-10:20 **5C1** **Yuta Hori**
Analysis of catalytic reaction mechanisms for the development of catalysts for hydrogen and methane oxidation by quantum chemical calculations

10:20-10:45 **5C2** **Kanami Sugiyama**
Theoretical Analysis of the Initial Process of GaN Crystal Growth by Using a Systematic Reaction Path Search

10:45-11:10 **5C3** **Jaewook Kim**
Holistic study on degradation mechanisms in blue OLED materials

11:10-11:35 **5C4** **Nawee Kungwan**
Excited state intramolecular proton transfer (ESIPT) from principal photophysics to the development of new chromophores and applications in fluorescent probes and luminescent materials

11:35-12:00 **5C5** **Satoshi Maeda**
Exploration of chemical reaction pathways for first-principles prediction of chemical reactions

Chair: Hiroki Uratani

14:00-14:25 **5C6** **Yasuteru Shigeta**
Computational studies on structure-function relationship of metalloproteins

14:25-14:50 **5C7** **Debashree Chakraborty**
A Universal Reaction coordinate for exploring the peptide permeation from "Direct" to "Endocytic" way by Umbrella Sampling method.

14:50-15:15 **5C8** **Ye Mei**
Reweighting Method for Free Energy Calculations in Condensed Phase

15:15-15:40 **5C9** **Mitsuo Shoji**
Water Oxidation Reactions in Natural and Artificial photosynthesis

15:40-16:05 **5C10** **Patchreenart Saparpakorn**
Binding Mode of Potent Acetylcholinesterase Inhibitors from Natural Products using Molecular Dynamics Simulations and Quantum Chemical Calculations

16:05-16:30 **5C11** **YunDong Wu**
Towards Effective Studies of Cyclic Peptides and Protein-Peptide Interaction-based Drug Design

16:30-16:55 **5C12** **Supa Hannongbua**
From QSAR to Deep Learning in Drug Design: Advancing Acetylcholinesterase Inhibitor Discovery

Room 4

Chair: Divya Nayar

9:55-10:20 **5D1** **Ayako Nakata**
Theoretical search for characteristic atoms in metallic nanoparticles by Large-scale DFT and statistical analysis

10:20-10:45 **5D2** **Susumu Yanagisawa**
Determination of the ionization energy and the electron affinity of organic molecular crystals from first-principles: dependence on the molecular orientation at the surface

10:45-11:10 **5D3** **GeunSik Lee**
Intercalated 2D Magnets for High Curie Temperature and Alloy-type Catalysts for High Efficiency: DFT study

11:10-11:35 **5D4** **Yun Hee JANG**
Organic Photodetectors Operating Under Strong Sunlight: Combining Machine Learning And Density Functional Theory For Molecular Design Of Photochromic n-Type Dopants Mixed With p-Type Organic Semiconductors

11:35-12:00 **5D5** **Koichi Yamashita**
First-Principles Calculations on Optical Properties and Defect Structures of Ge-Doped Sn Perovskites

Chair: Susumu Yanagisawa

14:00-14:25 **5D6** **Tran Phuoc Duy**
Understanding the G protein activation pathway through the Adenosine A2A receptor using PaCS-MD/MSM

14:25-14:50 **5D7** **Mariia Ivonina**
Exploring SARS-CoV-2 RNA Pseudoknot Dynamics and Drug Interactions: Insights from Molecular Dynamics and Energy Decomposition Analysis

14:50-15:15 **5D8** **Toshifumi Mori**
Elucidating the Conformational Dynamics of Proteins During Enzyme Catalysis

15:15-15:40 **5D9** **Divya Nayar**
Living Cell Soup: Biomolecular Self-Assembly to Nanomaterial Design

15:40-16:05 **5D10** **Hao Wang**
Modeling and analyzing rare event kinetics in complex systems

16:05-16:30 **5D11** **Toyokazu Ishida**
Insight into Catalytic Mechanism of GH11 Xylanase: ab initio QM/MM Modeling based on Neutron Structure

16:30-16:55 **5D12** **Yu Takano**
Quantum chemical evaluation of noncovalent interactions in proteins using the combination of ONIOM method and negative fragmentation approach including counterpoise correction

Reception Hall

9:40-9:55 ***Breaks***

12:00-14:00 ***Poster&Lunch***

16:55-17:15 ***Breaks***

22-Apr, Tuesday

12:00-14:00 ***Poster Presentation***

2P1 **Chou Ching Teng**
Mechanism understanding of catalyst morphology and support effects on N_2 activation in ammonia production: A DFT study

2P2 **Souvik Manna**
Integrated Supervised and Unsupervised Machine Learning Approach to Map the Electrochemical Windows Over 4500 Solvents for Battery Applications

2P3 **Aulia Sukma Hutama**
Molecular Dynamics Simulations of Water Adsorption and Dissociation on Yttria Surfaces

2P4 **Lan-Yun Chang**
Generative Modeling for Expanding Functional Group-Protein Complex Database to Overcome Structural Limitations

2P5 **Dae-Hwan Ahn**
Accurate Prediction of Core Excitation Energies for Transition Metals with Long-range Corrected Density Functional Theory including Multiple Gaussian Attenuated HF Exchange

2P6 **Thanawit Kuamit**
Density functional theory calculations of hydrogen adsorption on metal-ion doped 4N-divacancy defect GQDs and pristine GQDs

2P7 **Pham Long-Hung**
Quantitative Atomistic Graph: a high-throughput computational platform for prioritisation of allosteric and functional residues across the proteome

2P8 **Sangmin Lee**
Classical Model for Aqueous Proton Transport

2P9 **Beomgyu Kang**
Investigations on Li+ transport mechanisms in inorganic glassy solid electrolytes using machine learning potential

2P10 **Plotoon Nonthaphon**
Virtual Screening of Herbal Medicine Recipes as Acetylcholinesterase Inhibitors for Alzheimer Disease

2P11 **Yao Fu**
Predicting molecular dynamics bond force constants using graph neural network

2P12 **Wenlong Xi**
Effects of transition metal (Fe/Co/Ti) doping on intercalation properties and phase transformation of MoS2 as anode materials for sodium-ion batteries: A first-principles study

2P13 **Chimprasit Aunlika**
Roles of binding between diterpene lactone derivatives and the Main protease of the Severe Acute Respiratory Syndrome Coronavirus-2 by Molecular dynamics simulations and Quantum chemical calculations

2P14 Changhwan Ji
Effect of Strain Induced Crystallization on Mechanical Reversibility of Thermoplastic Elastomer

2P15 Hirobumi Mineo
Unidirectional pi-electron rotations for the helical-photo-dressed states in aromatic ring molecules

2P16 Tatsuhiro Nakanishi
Analysis of reaction path bifurcation utilizing Natural Reaction Orbital (NRO) method

2P17 Seokhyun Moon
DSMDock: A Unified Deep Learning Approach to Binding Pose and Affinity Estimation through Energy-Based Modeling

2P18 Gayoung Kim
Curvature-dependent lipid domain patterning in phase-separating liposomes

2P19 Viktor Khinevich
Enhancing Quantum Power Methods with Generalized Quantum Signal Processing

2P20 Seonghui Kim
Analysis of tracer diffusion confined in a dynamic network

2P21 Nahyun Chi
Evaluating Molecular Dynamics Approaches for Melting Point Prediction of Organic Crystals

2P22 Sanghoon Lee
The Effect of Intermolecular Edges in Graph Neural Networks

2P23 Ryuto Kambara
Exploring nonadiabatic dissociation of doubly-ionized OCS molecules via AIMD simulations

2P24 Pavinee Prapassornwattana
Computational Study of the Condensation of FUS Induced by Small Charged Molecules

2P25 Patrick Sutton
Mechanistic Insights into the Function of the Quaternary Ammonium Compound Transporter A (QacA) in Methicillin Resistant Staphylococcus aureus

2P26 Kyunghoon Lee
Extending the Automation of Reaction Profile Calculations: Applications to Realistic Chemical Reactions

2P27 NIHARIKA Keot
From Stability to Magnetism of bis-hydrated Mn(II) Complexes: A Computational Perspective

2P28 Saikat Hazara
Ortho-Para Conversion for H+ + H2 Collision in Low Temperature: A Fully Closed Coupled Time Dependent Wave Packet Study

2P29 Manisha Sharma
Equation-of-motion coupled-cluster with single, double and triple substitutions for studying ionization, double ionization, and one- and two-electron attachments: Computational implementation and some pilot applications.

2P30 Akash Gutal
Quasi-classical Trajectory Simulations of the CN^- + CH_3I Bimolecular Reaction using High Dimensional Neural Network Potentials.

2P31 Shubham Bajpai
Computational Insights into GPx-Like Activity and Charge Transfer in Chalcogen-Substituted Naphthalene and Perylene Derivatives

2P32 Bhrigu Chakraborty
Modified Bonobo Optimizer in the Global Optimization of Atomic Clusters

2P33 Xiao Xu
Non-Imprinted Polymers as Synthetic Antibodies for Protein Recognition: A Perspective from Molecular Dynamics Simulation

2P34 Yuqi Wang
Multi-reference Random Phase Approximation via Diagrams

2P35 Nupur Jain
Efficient Machine Learning for Yield Prediction in a Transition Metal Catalyzed meta-C(sp2)–H Bond Activation Reaction

2P36 Gargee Kashyap
Automated Selection of Molecular Fingerprints for Dataset-Specific Representation for Chemical Datasets

2P37 Chen-Wen Wang
Franck-Condon study of vibrational aspects for ESIPT dyes of 2-(20- hydroxyphenyl)-3,30-dimethylindole (HDMI)

2P38 Cheng-Han Liu
Sequence-Dependent Interaction Mechanism in Vancomycin Binding to a DNA Aptamer: A Molecular Dynamics Study

2P39 Chi-Chi Wu
Insights into the difference between conventional (O-H) and unconventional (S-H) excited-state intramolecular proton transfer: A combination of theoretical and experimental approach

2P40 Guan-Fang Wang
Exploring the Secondary Nucleation Mechanism on Fiber Surfaces Using Coarse-Grained Molecular Dynamics Simulation

2P41 Youhao Shang
Constraint Phase Space Formulations for Finite-State Quantum Systems

2P42 Yingjie Pan
Design of Novel Pathways for Production of Bio-Based Chemicals in Multi-Enzyme Cascades

23-Apr, Wednesday

12:00-14:00 ***Poster Presentation***

3P1 **Rounak Nath**
Unraveling the Regioselective Reaction Mechanism of Gentisic Acid Catalyzed by SDO Enzyme

3P2 **Maitreyee Sarkar**
Quantum Simulations of Chemical Reactions: Achieving Accuracy with NISQ Devices

3P3 **Baihua Wu**
Nonadiabatic Field on Quantum Phase Space

3P5 **Dae-Hwan Ahn**
Theoretical Investigation of Solvent and Relativistic Effects on the Optical Spectra of a Complex Containing Hg2+ Ion

3P6 **Wilasinee Santiwarodom**
Density Functional Theory Study of CO_2 Conversion to CO via Metal-N_4-Schiff Base Complexes

3P7 **Fungerlings Achim**
Effect of surface transformation and oxygen stoichiometry on the oxygen evolution reaction activity of nickelates

3P8 **Sirilak Kongkaew**
How Can N-Doped/BN-Modified Triphenylene-Graphene Catalysts Efficiently Electroreduce CO2 into Valuable Chemicals?

3P9 **Seungwon Kim**
A Bayesian Committee Machine Potential for Oxygencontaining Organic Compounds

3P10 **Todsaporn Duangjai**
Discovery of Furochochicines as Potent JAK2 Inhibitors for Cervical Cancer: Combining Machine Learning-Based QSAR and Experimental Validation

3P11 **Shebual Sebastian**
TD-DFT Challenge: Can modern spin scaled double hybrids overcome the overestimation trend in BODIPY dyes? Answers and recommendations from a TD-DFT benchmarking study

3P12 **JEONGSIK LEE**
Integrating Docking, Molecular Dynamics, and Multi-Condition Pareto Analysis with DNA-Encoded Library

3P13 **Risa Amano**
First-principles calculations of optical force and torque on C3H6 molecule

3P14 **Seungwon Jeong**
Highly Accurate Predictive Polarizable Force Field for the Lithium-Ion Battery Electrolytes

3P15 **Fadjar Mulya**
DFT Study of Na ion/atom Adsorption on GQDs for Battery Applications

3P16 **Ryusei Nishimura**
Divide-and-Conquer-Based Geometry Optimization of Non-Local Excited States

3P17 JiHoon Kim
Highly reliable and large-scale simulations of promising argyrodite solid-state electrolytes using a machine-learned moment tensor potential

3P18 Muhammad Rizwan Khan
Interplay Between Intrinsic Structural Defects and Optoelectronic Properties in Semi-Heusler Gapped Metals

3P19 JunHo Seok
Catalytic Activity of 2D Carbon Allotropes: The Critical Role of Local Structural Configurations in HER/OER

3P20 Wonho Zhung
Chemical Knowledge-guided Generative Modeling for Multi-objective Structure-based Drug Design

3P21 Ada S Quinn
PolyConstuct: a python module to prepare arbitrary polymers for molecular dynamics simulation

3P22 Miftahussurur Hamidi Putra
The Mechanistic Process of Catalyst Degradation on RuPt-Based Photochemical Molecular Devices: From Theoretical Perspective

3P23 Patigo Apinya
Binding study of the 4-isochromanone derivatives as acetylcholinesterase (AChE) inhibitors by computational study and ADMET predictions

3P24 Yoosang Son
Time-domain Analysis of Electron Transfer

3P25 Ariel Cambridge Jones
Describing Excited-State Non-Covalent Interactions with Time-Dependent DFT

3P26 Yeonho Song
Characterization of the DNA Catenane: A Molecular Dynamics Simulation Approach

3P27 Witayapaisitsan Naphol
Mechanistic Insights into Ru-S Complex-Catalyzed C-H Silylation and Borylation of N-heteroarene: Distinct Bonding Interactions

3P28 Charlie Ruffman
Dynamic Liquid Metals as Catalysts for Selective CO2 Reduction

3P29 Shota Tsuru
Nuclear quantum effects have a significant impact on UV-Vis absorption spectra of chromophores in water

3P30 Shubham Kumar
Dynamic Slowdown and Spatial Correlations in Viscous Silica Melt: Perspectives from Dynamic Disorder

3P31 Priya Dey
Relaxation dynamics measure the aggregation propensity of amyloid-β and its mutants

3P32 Kenji Okada
Diphenoquinone as a Novel Building Block of Singlet Fission Chromophores

3P33 Lintai Da
Mechanistic Investigation and Rational Design of Glycotransferase

3P34 Mridula choudhary
Computational Insights into Titanium and Lithium-Catalyzed Hydroboration: Mechanistic Pathways and Reactivity Trends

3P35 Xiangsong Cheng
A New Class of the Exact Population Dynamics Expression for Pure Two-State Systems and a New Propagator for the Nonadiabatic Force in Nonadiabatic Field

3P36 Qing Zeng
CPconf_score: A Deep Learning Free Energy Function Trained Using Molecular Dynamics Data for Cyclic Peptides

3P37 Hsin-Ying Chang
Giant virus-host prediction using machine-learning methods

3P38 Jen-Shiang Yu
Characterization of Enol Ether Intermediates in the Intramolecular Stetter Reactions by DFT and Kinetic Simulations

3P39 Jia-Xian Yin
Exploring CXCR3-CXCL11 Interactions: Insights from Molecular Dynamics Simulations

3P40 Karen Sargsyan
Non-Conservative Forces and Nontrivial Thermodynamics Produced by Machine Learned Potentials

3P41 Luis Vasquez
Towards Rigorous Interconnection Between Polarization-Detected and Population-Detected Signals

3P42 Jinda Luo
Halide Superionic Conductors with Non-Close-Packed Anion Frameworks

25-Apr, Friday

12:00-14:00 ***Poster Presentation***

5P1 Sandeep Kumar Reddy
Computational studies of structure and dynamics of one-dimensional supramolecular polymers

5P2 Bingqi Li
Nonadiabatic Field with Novel Hill Window Functions on Quantum Phase Space

5P3 Yingjin Ma
Large-scale fragmented quantum chemical calculation with fault-tolerant

5P4 Patrik Chandra
Glycerol Hydrodeoxygenation into Propanediols Over Platinum-modified Reduced Graphene Oxide Catalyst: A DFT Study

5P5 **Norraset Cheevatanomsak**
Insights into the product selectivity in iridium-catalyzed transfer dehydrogenation of alkane

5P6 **Juan Felipe Huan Lew Yee**
Natural Orbital Functional Theory for Large Correlated Systems

5P7 **Minho Kim**
Phase transition drives anomalous capacitance peak in aqueous electric double layer

5P8 **Rei Oshima**
Direct minimization method for SCF solution using Givens rotation and error backpropagation

5P9 **Rathawat Daengngern**
Structural Stability of Proline in the Gas and Solution Phases by Quantum Chemical Calculations

5P10 **Yuichiro Oda**
Quantum chemical analysis of noncovalent interactions in protein secondary structures using Negative Fragmentation Approach

5P11 **Hyeok Jae Lee**
Substructure-aware and Exaplainable Machine Learning for Blood brain Barrier Permeability

5P12 **Pavee Apilardmongkol**
Next-Generation Catalysts for Ethylene Polymerization: Theoretical Design Based on Nickel Diimine Catalysts

5P13 **Jae Hun Seol**
Strategic Ligand-induced Electronic Structure Modulation for Enhanced Nitrogen Reduction Reaction Selectivity in Transition Metal Phthalocyanines

5P14 **Billy Joseph Williams-Noonan**
Antiseptic and Lipid Transport Pathways via the QacA Efflux Pump: Insights from Metadynamics Simulations

5P15 **Jana Radakovic**
Stand-alone target-focused natural language embeddings as source of chemical information for predicting physico-chemical properties

5P16 **Lihao QU**
Accelerating Reaction Space Projector (ReSPer) by Combinatorial Optimization Method: Validations and Applications to Organic Chemical Reactions

5P17 **Da Bean Han**
Machine Learning-guided Electronegativity for Organic Molecules

5P18 **Kotomi Nishikawa**
Nuclear Quantum Effects on the Intramolecular Hydrogen Bonds in Biuret and Biguanide Analyzed by PIMD Method

5P19 **Hyungshick Park**
Screening and Correlated Ion Diffusion in Lithium-Doped Ionic Liquids

5P20 **Amy Christina Hancock**
How Robust Are TD-DFT Methods And Ground-State Dispersion Corrections For Noncovalent Interactions In Higher-Lying Excited States Of Aromatic Dimers?

5P21 **Miu Ashiba**
Isomer effect on the positron bindings to halogenated hydrocarbons

5P22 **Namsopa Chonticha**
Virtual Screening of "Styrax tonkinensis" Targeting Acetylcholinesterase by Computational Calculations

5P23 **Shengzhou Li**
Large-scale DFT and machine learning assisted theorectical investigation on the interface in supported nanoparticles

5P24 **Satoi Wada**
Non-adiabatic Molecular Dynamics Study on the Photo-excited Reaction of Ortho-nitrophenol in the Gas Phase

5P25 **Vic Austen**
A Theoretical Investigation into Water Oxidation Catalyzed by Alloyed Pentanuclear Complexes

5P26 **Nilson Kunioshi**
Quantum Chemical Analysis of the Hydrolysis Reactions of Phospholipids

5P27 **Manussada Ratanasak**
Revisiting the Mechanism of Fluoroacetate Dehalogenase-Catalyzed Degradation of Fluorocarboxylic Acid

5P28 **Ryoma Shimizu**
Prediction of Inhibitory Activity of Carbonic Anhydrases Using Free Energy Perturbation Simulations

5P29 **Sagar Ghorai**
Towards reaction vessel mimicry: Machine learning assisted automated exploration of alkene and alkyne polymerization

5P30 **Chen Yang**
Advances in Neural Networks for Electronic Structure Calculations

5P31 **Brandon MezaGonzalez**
Probing Reaction Mechanisms on a Membrane Using Metadynamics Simulations

5P32 **Arpita Varadwaj**
Band Gap Engineering and Stability Analysis of Transition Metal Dichalcogenide and MXene Heterostructures

5P33 **Sayon Satpati**
A Quantum Chemical Approach to Hydrocarbon Database: Spectral Predictions and Characterization for Astrochemical Research

5P34 **Botao Dai**
Accurate Structure Prediction for Cyclic Peptides Containing Proline Residues with High-Temperature Molecular Dynamics

5P35 **Sonaldeep Halder**
Dynamic Ansatz Construction Utilizing Generative Machine Learning for Noisy Quantum Hardware

5P36 **Kazuaki Kuwahata**
Nuclear quantum effects on phase transitions of high-pressure ice

5P37 Liang-Ting Wu
Combined machine learning and computational protocols to predict electrolyte behavior and SEI formation in Li-metal batteries

5P38 Wei-Hsiang Wang
Human Serum Albumin Interactions with Fluorescent Probes: A Simulation Study

5P39 Zhong-Lun Li
Machine Learning and First-Principles Insights into Optimizing Multi-Component Electrolytes for Lithium-Metal Batteries

5P40 Stanislav Kedžuch
Single reference coupled cluster theory for systems with strong correlation extended to excited states

5P41 Jingxian Yu
Ultrafast knock-off Li+ diffusion and subtle structural evolution of Li5V3O8 anode in lithium-ion batteries

5P42 Longfei Chang
Quantum-assisted variational quantum Monte Carlo

5P43 Yixi Zhang
REANN-Z: An Efficient Universal Neural Network Potential with Element Embedding