June 17 (Mon)

13:50 **Opening address**

Chairperson: Josef Noga

14:00 OI-01 **Seiichiro Ten-no**
"Projective Transcorrelation Theory"

14:25 OI-02 **Zsuzsanna Mihalka**
"Geminal-based wavefunctions with explicitly correlated correction"

14:50 OI-03 **Hiroyuki Nakashima**
"Recent highly accurate calculations of small atoms and molecules by solving the Schrödinger equations with the free complement theory"

15:10 **Coffee break**

Chairperson: Yuki Kurashige

15:30 OI-04 **Jan Brandejs**
"Generating coupled cluster code for modern distributed memory tensor software"

15:55 OI-05 **Masaaki Saitow**
"An accurate, reduced-scaling wave function theory for excited states"

16:20 OI-06 **Libor Veis**
"Variational quantum eigensolver boosted by the adiabatic connection"

16:45 OI-07 **Wataru Mizukami**
"Developing Methods to Bridge the Gap Between Quantum Computers and Classical Computers in Electronic Structure Calculations"

17:05 OI-08 **Yuta Mizuno**
"Quantum Computing for Complex Chemical Systems Analysis"

18:30 **Welcome Reception**

June 18 (Tue)

Chairperson: Hiromi Nakai

9:00 OII-01 **Petr Bouř**
"Raman optical activity in and out of resonance: Interpretation through computational chemistry"

9:25 OII-02 **Tokuei Sako**
"Symplectic integrator approach to temporal-mode selective light-matter interaction"

9:50 OII-03 **Michal Repisky**
"Modern Exact Two-Component Hamiltonians for Relativistic Quantum Chemistry and Physics: Two-Electron Picture Change Corrections Made Simple"

10:15 OII-04 **Stanislav Komorovský**
"Relativistic theory of pNMR and EPR"

10:40 **Coffee break**

Chairperson: Jiří Pittner

11:00 OII-05 **Lukas Konecny**
"Relativistic linear response quantum electrodynamical density functional theory"

11:25 OII-06 **Tsuyoshi Kato**
"Density functionalization of Kohn-Sham potential"

11:45 OII-07 **Takao Tsuneda**
"Reactive intramolecular electrostatic force:Bridging electronic and potential energy frameworks"

12:05 OII-08 **Hiromi Nakai**
"Recent Advances in Divide-and-Conque Non-local Excited-State Calculation Method using Dynamical Polarizability"

12:25 **Lunch break**

13:30 **Poster Session I**

Chairperson: Hirofumi Sato

15:00 OII-09 **Miroslav Medveď**
"Computational Insights into Molecular Photochromism of Iminothioindoxyls"

15:25 OII-10 **Nissrin Alharzali**
"Unravelling the atmospheric degradation of pesticides using computational chemistry tools"

15:50 OII-11 **Azusa Muraoka**
"Charge Separation Process in BTAx Nonfullerene Organic Solar Cells"

16:10 **Coffee break**

Chairperson: Jan Řezáč

16:30 OII-12 **Yasuteru Shigeta**
"Theoretical Analysis on Formation Process and Stability of 3D Domain Swapping Proteins"

16:50 OII-13 **Jiří Kessler**
"Vibrational optical activity modelling of biomolecular systems"

17:15 OII-14 **Seiji Komeda**
"Interactions of in vivo anticancer-active dinuclear platinum(II) complexes with biomolecules"

17:40 OII-15 **Jaroslav Burda**
"The Description of the Reactions in Solutions with Constant pH; Ab initio/DFT approach"

June 19 (Wed)

Chairperson: Jaroslav Burda

9:00 OIII-01 **Jiří Pittner**
"Molecular dynamics with non-adiabatic and spin-orbit effects: theory, application, and machine learning"

9:25 OIII-02 **Yuki Kurashige**
"Spin Transitions and Relaxations in Non-adiabatic processes"

9:45 OIII-03 **Toshiyuki Takayanagi**
"Theoretical studies on positron binding in molecules"

10:05 OIII-04 **Tetsuya Taketsugu**
"Exploring Chemical Reaction Mechanisms and Dynamics with Quantum Chemical Tools: The Reaction Space Projector and Natural Reaction Orbital Methods"

10:25 **Coffee break**

Chairperson: Tomáš Bučko

10:45 OIII-05 **Jan Řezáč**
"Happy marriage of semiempirical quantum chemistry and machine learning"

11:10 OIII-06 **Hajime Torii**
"Elucidating the Characteristics of Halogen Bonding through Analyses of Electron Densities"

11:35 OIII-07 **Hirofumi Sato**
"Molecules in condensed systems: a chemical reaction and interactions with electromagnetic fields"

Chairperson: Jun-ya Hasegawa

11:55 OIII-08 **Jan Hrušák**
"Bridging Continents: Exploring the Global Landscape of Research Infrastructures (RIs) and Collaborative Opportunities"

12:20 **Lunch break**

13:30 **Poster Session II**

Chairperson: Jun-ya Hasegawa

15:00 OIII-09 **Satoshi Maeda**
"Ab Initio Exploration of the Pathways of Chemical Reactions"

Chairperson: Zdeněk Havlas

15:25 OIII-10 **Yasuhiro Kobori**
"Photoinduced spin entanglement and decoherence in triplet pairs"

15:50 OIII-11 **Hiroyuki Tamura**
"Combined Electronic Structure and Quantum Dynamical Analysis of Charge and Exciton Dynamics in Molecular Assemblies"

16:15 OIII-12 **Alexandr Zaykov**
"Quo Vadis, Singlet Fission?"

18:30 **Banquet**

June 20(Thu)

Chairperson: Shigeyoshi Sakaki

9:00 OIV-01 **Michal Straka**
"Hydrogen bonds to M(I) coinage metals. Experiment and theory"

9:25 OIV-02 **Agnieszka Stanczak**
"Unraveling tyrosinase reaction mechanism: interplay between experiment and theory"

9:50 OIV-03 **Miho Hatanaka**
"A descriptor database for metal-phosphorus complexes to evaluate the catalytic abilities using machine learning"

10:10 OIV-04 **Yasutaka Kitagawa**
"Theoretical Study on Redox Potential Control of Iron-Sulfur Cluster by Hydrogen Bonds"

10:30 **Coffee break**

Chairperson: Masahiro Ehara

10:50 OIV-05 **Jiří Brabec**
"Electronic structure of the highly-entangled polyradical nanographene with coexisting strong correlation and topological frustration"

11:15 OIV-06 **Ivan Stich**
"Quantum Monte Carlo study of straintronic response of 2D materials: monolayer phosphorene and MoS_2"

11:40 OIV-07 **Tomomi Shimazaki**
"Theoretical Study of Dielectric-Dependent Density Functional Theory and Molecular Passivation Effect on Lead-Free Tin Perovskite Surface Defects"

12:00 OIV-08 **Takahito Nakajima**
"Our Recent Research Progress on Materials Simulations and Informatics"

12:20 **Lunch break**

Chairperson: Ivan Stich

13:30 OIV-09 **Tomáš Bučko**
"Efficient calculation of fully anharmonic activation free energies at multiple electronic structure levels"

13:55 OIV-10 **Ryosuke Jinnouchi**
"First-principles electrochemistry: machine learning-aided free energy computations"

14:20 OIV-11 **Ayako Nakata**
"Large-scale DFT calculations on size- and site-dependences of electronic structures in metallic nanoparticle catalysts"

14:40 OIV-12 **Mitsutaka Okumura**
"Theoretical Study on TiOOH Production over Au/TiO_2 Catalyst"

15:00 OIV-13 **Masahiro Ehara**
"Electronic Structures and Photophysical Properties of Metal Nanoclusters"

15:20 **Closing remark**

June 18 (Tue) Poster Session I

PI-01	Kaho Nakatani	Spin symmetry in the group function theory
PI-02	Hiroshi Nakatsuji	Bird's-eye view of the Free Complement Theory for solving the Schrödinger equation
PI-03	Kazuma Uemura	Local N-electron valence state perturbation theory using pair-natural orbitals based on localized virtual molecular orbitals
PI-04	Stanislav Kedzuch	Extending coupled cluster theories with static correlation
PI-05	Chinami Takashima	Acceleration of local unitary transformation in two-component relativistic calculation based on element-based algorithm and parallel implementation
PI-06	Hajime Miyamoto	Theoretical study on singlet fission process in one-dimensional aggregate systems considering position-dependent intermolecular electronic couplings
PI-07	Manaya Kawasaki	Theoretical Study on Electronic Excited States of a Gallylene Baring a Phenalenyl-Based Ligand
PI-08	Hiroto Komuro	Exploration of photochemical reaction paths in N-salicylideneaniline crystal
PI-09	Vladimir Malkin	Transmission of spin-polarization by π-orbitals
PI-10	Kenichiro Saita	A theoretical study on the conrotatory and disrotatory ring-opening pathways of 1,3-cyclohexadiene
PI-11	Debora Misenkova	Relativistic theory of the EPR g-tensor
PI-12	Katsuki Miyokawa	Ab initio study of electron spin-lattice relaxation of triplet oligoacenes
PI-13	Monika Gešvandtnerová	Isobutanol to linear butenes conversion: importance of dynamic effects addressed by AIMD
PI-14	Ryuto Kambara	AIMD study on nonadiabatic dissociation processes of OCS2+
PI-15	Yukun Bai	Integrating Quantum Chemical Calculations and Molecular Dynamics Simulations for the Crosslinking Process of Cyanate Resin
PI-16	Ryo Okabe	Elucidation of dissolution state and excited state of a fluorescent probe in a lipid bilayer
PI-17	Manabu Kanno	Near-Infrared-Induced Conversion from Polyhydroxy Fullerenes to Graphene Flakes as a Seed for Carbon Nanotubes

PI-18	Sheng-Han Yang	Constructing extensive quantum chemistry calculated interaction energy dataset for machine learning potential
PI-19	Masami Lintuluoto	Calcium oxalate flocculation under peptide and phosphorylated peptide
PI-20	*Cancelled*	
PI-21	Ren Yamada	Extension of the virtual ligand method to arsenic ligands
PI-22	Akihiro Mutsuji	Theoretical analysis of electron self-exchange reactions of transition metal complexes by an energy decomposition and extrapolation scheme and potential-crossing optimization
PI-23	Noriyuki Takai	Quantitative electronic theory analysis of Suzuki-Miyaura cross-coupling reaction
PI-24	Shinichi Suda	Development of Virtual Ligands for 1,2-Bis(diphenylphosphino)ethane and Its Derivatives
PI-25	Wieslaw Nowak	New insights in insect sodium channels functioning from a theoretical perspective
PI-26	Mai Fujiwara	Effect of N-glycosylation and metal ions on catalytic activity and substrate specificity of serine protease Neuropsin (KLK8)
PI-27	Nina Buckova	Analysis of interactions determining the intricate properties of water
PI-28	Kanami Sugiyama	Analytical optimization method for molecular orientation using distance geometry
PI-29	Gen Ogawa	Ab initio DC-PBC method: Development of computational chemistry platform for amorphous materials
PI-30	Katarína Skladanová	Adsorption of benzene on graphene explored using ab initio molecular dynamics and machine learning force fields
PI-31	Jewel Hossen	Theoretical study of anodic chlorine evolution reaction on carbon nanomaterial-supported Pt-complex catalyst
PI-32	Andrey Lyalin	Two-dimensional layers of boron: on the metal and with the metal
PI-33	Naoka Amamizu	Difference in Spin Structure of Metal-Organic Frameworks between Cluster Model and Periodic System
PI-34	William Dawson	Complexity Reduction in Density Functional Theory: Locality in Space Energy
PI-35	Aditya Wibawa Sakti	Effects of Solvent and Ion Interactions to the Polysulfide Diffusion in Li-S Battery Electrolyte Models

PI-36	Shogo Morisaki	The development of the reactive force field fitting program “reaxfit” and its application to Co surface reaction systems
PI-37	Masatsugu Nishida	DC-xTB-MD: A general-purpose, enormously large-scale quantum chemical calculation method
PI-38	Mai Otake	Theoretical Study on Defects in Sn/Ge Double Perovskite Solar Cells Using First-Principles Calculations
PI-39	Shoya Kondo	Global search for molecular crystal structures under high pressure by interfacing AFIR and GAFF

June 19 (Wed) Poster Session II

PII-01	Yusaku Kurokawa	Highly accurate analytical solution of the Schrödinger equation of He atom: New trial
PII-02	Yutaro Otani	Development of Multireference perturbation theory based on the doubly-occupied CI wavefunction: A DOCI-Fock operator formalism
PII-03	Viktor Khinevich	Enhancing Quantum Computations with the Synergy of Auxiliary Field Quantum Monte-Carlo and Computational Basis Tomography
PII-04	Rei Oshima	Development of SCF convergence method combining Givens rotation and error back propagation method
PII-05	Alexandr Zaykov	Point of Discussion: SPARC and Singlet Fission
PII-06	Tetsuri Takami	Theoretical Study on Vibronic Structures of Carbon Cluster Anions C6- and C6H-
PII-07	Tohru Taniguchi	Comparison of Calculated and Observed Raman Optical Activity Spectra of Deuterated Glucoses in Water
PII-08	Kaichi Shimada	Theoretical study on electronic structures and properties of open-shell molecular systems involving azulene units
PII-09	Mitsuhiro Nishida	Theoretical study on the impact of heteroatom substitution on single-molecule electrical conductivity
PII-10	Olga Malkin	Distinguishing “Through-Space” from “Through-Bonds” Contribution in Indirect Nuclear Spin-Spin Coupling
PII-11	Haruka Araragi	Electronic structure calculations for NTz-based acceptor molecules non-fullerene organic solar cells
PII-12	Pei Zhao	Theoretical Insights into Photoluminescence of Functionalized Carbon Nanotubes
PII-13	Kentaro Hino	Machine learning potential via matrix product representation: Friendly multiplication with many-body wavefunction
PII-14	Takafumi Shiraogawa	Real-time time-dependent density functional theory (RT-TDDFT) simulations of quantum systems interacting with orbital angular momentum (OAM) light

PII-15	Sitorabonu Musoeva	Impact of DFT Functionals for Trajectory Surface Hopping: The Case of Thymine Photorelaxation
PII-16	Hiroki Uratani	Non-adiabatic molecular dynamics method using electronic configurations as many-electron basis set
PII-17	Takuro Tsutsumi	Elucidations of Dynamical Reaction Processes based on Reaction Space Projector (ReSPer)
PII-18	Yi-Ta Lin	The application of Deep Potential Molecular Dynamics for methane
PII-19	Takumi Koshiba	Potential energy estimation by Gaussian process regression for acceleration of the structure-based Gaussian expansion processes
PII-20	Florian Lemken	Theoretical Study on Catalytic CO2 Reduction with Heptacoordinated Polypyridine Complexes
PII-21	Junki Sugimura	Theoretical Study on CO2 Fixation Catalyzed by Polyoxometalate
PII-22	Ken Hirose	Development of Virtual Lewis Acid for in silico Design of Lewis Acid Catalyst
PII-23	Yamato Ueno	Computational Substrate Design to Achieve a Potential Side Reaction within the Reaction Path Network and Experimental Demonstration: Aryl Carboxylation of Alkenes
PII-24	Sara Suzuki	Reaction enhancement by microscopic solvation: Z-(allyloxycarbonyl)methyl radical cyclization reaction
PII-25	Tatsuhiro Nakanishi	Natural reaction orbital (NRO) analysis for understanding reaction path bifurcation from electronic theory perspective
PII-26	Ryusei Morimoto	Theoretical investigation of the mechanism for NH3-SCR over Cu-CHA
PII-27	Wataru Kanna	Reaction Development Utilizing Crossing Point Search for Single Electron Transfer Steps in Catalytic Olefin Aminocarboxylation with CO2
PII-28	Kazuki Honjo	Theoretical study on the effect of surrounding environment on electronic states around reaction active center of nitrogenase

PII-29	Dávid Vrška	Fully anharmonic finite temperature thermodynamic calculations at the CCSD(T) and many DFT levels of the gas-phase dimerization of formic acid
PII-30	Ryohei Kishi	Theoretical Study on Electronic Structures and Response Properties of π-Stacked Multimers of Antiaromatic Molecules
PII-31	Airi Kawasaki	Warning! The negative divergence of the stress tensor isn't always the Ehrenfest Force
PII-32	Ryota Sugimori	Analysis of electronic structures of antiaromatic molecular π-dimers based on the multi-reference perturbation theory calculations using the diabatic basis representations
PII-33	David Samuel Rivera Rocabado	Introducing the Electronic Structure Decomposition Approach for CO Adsorption and Activation on Ru/α-Al2O3(0001)
PII-34	Yasutaka Hamada	A DFT study of propylene epoxidation on Ti-containing material supported Au cayalysts.
PII-35	Masato Kobayashi	Mapping between amorphous and crystal structures based on metastable crystal structure database and persistent homology
PII-36	Tomoya Shiota	Accelerating High-Entropy Alloy Catalysts Screening using Monometallic Data and Descriptors from Neural Network Potentials
PII-37	Kai Oshiro	Theoretical investigation of the alkali metal poisoning tolerance mechanism of CeO2 containing Fe and H2SO4 additives
PII-38	Chinami Okamura	Theoretical studies on the reaction mechanism of Li-mediated ammonia synthesis
PII-39	Ram Kinkar Roy	Is the Oscillator Strength Computed by Spin-Flip Long-Range-Corrected TDDFT (SF-LC-TDDFT) Method a Reliable Parameter to Investigate Fluorescence Quenching?