TACC2023 Scientific Program

Monday, September 4, 2023

13:00 -	**Registration Desk Open** (Centennial Hall, School of Medicine)
Opening Session (Large Auditorium) Chair: Tetsuya Taketsugu	
15:00 - 15:30	**Opening Ceremony**
15:30 - 16:15	**4PL-1. Plenary Lecture**: *Eiichi Nakamura* "Cinematic Chemistry." Transforming Chemistry from Thermodynamics to Statistical Mechanics by VT-VV SMART-EM Imaging
16:15 - 17:00	**4PL-2. Plenary Lecture**: *Mark S. Gordon* The Effective Fragment Potential: An *Ab Initio* Force Field
18:00 - 20:00	**Welcome Reception** (Poplar-kan, Sapporo Beer Garden)

Tuesday, September 5, 2023

8:30 -	**Registration Desk Open** (Frontier Applied Science Bldg.)		
Plenary Lecture (Large Auditorium) Chair: Hiromi Nakai			
9:00 - 9:45	**5PL-1**: *Gustavo E. Scuseria* Adventures in Strong Correlation		
9:45 - 10:15	**Coffee Break**		
	5A1. Theory, Method, & Computation (Large Auditorium) Chair: Chao-Ping Hsu	**5B1. Machine Learning & Informatics** (Suzuki Hall) Chair: U. Deva Priyakumar	**5C1. Condensed Phase** (Seminar Room 2) Chair: Hirofumi Sato
10:15 - 10:30	**5A1-1I**: *Tomas Kubar* Simulation of reactions in biomolecular complexes: Blending the flavors	**5B1-1I**: *Keisuke Takahashi* Materials Informatics: Perspective and Opportunities	**5C1-1I**: *Akihiro Morita* Transport and Reactions at Liquid Interfaces
10:30 - 10:45			
10:45 - 11:00	**5A1-3I**: *Ana-Nicoleta Bondar* Graph algorithm and graphical user interface to dissect mechanisms of membrane receptor activation	**5B1-3I**: *Johannes Hachmann* Making Data Science Work for Chemistry	**5C1-3I**: *Amalendu Chandra* Nonlinear one- and two-dimensional vibrational spectroscopy of aqueous interfaces with surfactants from a combination of simulations and quantum calculations
11:00 - 11:15			
11:15 - 11:30	**5A1-5I**: *Ksenia Bravaya* Simulating electron-mediated processes in proteins: from mechanistic predictions to observables	**5B1-5I**: *Yousung Jung* AI-Enabled Synthesis Predictions for Molecules and Materials	**5C1-5C**: *Kenji Iida* Development of Theoretical Approach for Heterogeneous Solid-Liquid Interface Under Bias Voltage
11:30 - 11:45			**5C1-6C**: *Yoyo Hinuma* Searching maximally orthogonalized supercells with given size for an arbitrary crystal
11:45 - 12:00	**5A1-7I**: *Vera Krewald* The Marcus dimension: identifying the nuclear coordinate for electron transfer from *ab initio* calculations	**5B1-7C**: *Mikael Kuwahara* CADS - Data Analyzing, Manipulation and Machine Learning Made Easy and Accessible	**5C1-7I**: *Yasuteru Shigeta* Computational studies on inhibition mechanism of some metalloproteins
12:00 - 12:15		**5B1-8C**: *Erickson Fajiculay* Memory efficient Incremental Kernel Ridge Regression with a smart chunking strategy	
12:15 - 13:45	**Lunch Break**		

Tuesday, September 5, 2023

Plenary Lecture (Large Auditorium) Chair: Emilio Martinez-Nunez			
13:45 - 14:30	**5PL-2**: *Satoshi Maeda* *Ab initio* reaction discovery through forward and backward kinetic simulations		
14:30 - 15:00	**Coffee Break**		
	5A2. Theory, Method, & Computation (Large Auditorium) Chair: Cheol Ho Choi	**5B2. Chemical Reaction & Dynamics** (Suzuki Hall) Chair: Miho Hatanaka	**5C2. Excited State & Spectroscopy** (Seminar Room 2) Chair: Yuriko Aoki
15:00 - 15:15	**5A2-1C**: *Masanori Tachikawa* Quantum Monte Carlo study on positron binding to atomic anion dimers	**5B2-1I**: *Thomas Weymuth* Automated and Interactive Exploration of Chemical Reaction Networks	**5C2-1I**: *Chaoyuan Zhu* Global switching algorithm for trajectory surface hopping molecular dynamics simulation within time dependent density functional theory
15:15 - 15:30	**5A2-2C**: *Daisuke Yoshida* Positron binding and annihilation properties of hydrogen bonded binary molecular clusters		
15:30 - 15:45	**5A2-3I**: *Kimihiko Hirao* The core ionization energies calculated by Delta SCF and Slater's transition state theory	**5B2-3I**: *Emilio Martinez-Nunez* Automated reaction mechanism discovery with AutoMeKin2021	**5C2-3C**: *Aaditya Manjanath* Probing chemical reaction dynamics through excited-state time-dependent *GW* simulations
15:45 - 16:00			**5C2-4C**: *Andrea Bonvicini* Quantum electrodynamics theory and computational implementation of the hyper-Rayleigh scattering optical activity spectroscopy
16:00 - 16:15	**5A2-5I**: *Piotr Piecuch* Converging High-Level Coupled-Cluster Energetics via Semi-Stochastic, Selected-CI-Driven, and Adaptive CC(P;Q) Approaches	**5B2-5I**: *Hiroko Satoh* Development and applications of methods for efficient use of large reaction route networks	**5C2-5C**: *Yasuhiro Ikabata* Controlling factors for the minimum energy conical intersection: Theoretical investigation and application
16:15 - 16:30			**5C2-6C**: *Henry K. Tran* Anharmonic Vibrational Structure and Spectra using Vibrational Heat-Bath Configuration Interaction
16:30 - 16:45	**5A2-7I**: *Seiichiro L. Ten-no* Selected coupled-cluster with F12 corrections	**5B2-7I**: *Woo Youn Kim* Efficient prediction of chemical reaction paths via graph theory and machine learning	**5C2-7I**: *Kiyoshi Yagi* Anharmonic Vibrational Calculations of Biomolecules and Polymers Based on Local Coordinates
16:45 - 17:00			
17:00 - 19:00	**5Po. Poster Presentation 1 (Centennial Hall, School of Medicine)**		

Wednesday, September 6, 2023

8:30 -	**Registration Desk Open** (Frontier Applied Science Bldg.)		
Plenary Lecture (Large Auditorium) Chair: Daniel M. Zuckerman			
9:00 - 9:45	**6PL-1**: *David M. Leitner* Modeling thermal transport in molecules		
9:45 - 10:15	**Coffee Break**		
	6A1. Theory, Method, & Computation (Large Auditorium) Chair: Satoshi Maeda	**6B1. Biomolecule & Drug Design** (Suzuki Hall) Chair: Yasuteru Shigeta	**6C1. Chemical Structure & Interaction** (Seminar Room 2) Chair: Kaito Takahashi
10:15 - 10:30	**6A1-1I (ICReDD Lect.):** *Frank Neese* What is a Multireference State?	**6B1-1I**: *Ayori Mitsutake* Investigating Protein Dynamics Using Relaxation Mode Analysis	**6C1-1I**: *Takako Kudo* Theoretical study of Si/C mixed analogues of some hydrocarbons
10:30 - 10:45			
10:45 - 11:00	**6A1-3I**: *Debashree Ghosh* Machine learning configuration space and matrix product state ansatz	**6B1-3I**: *Daniel M. Zuckerman* Rate constants for complex systems from weighted ensemble simulation: Successes and challenges	**6C1-3I**: *Chin-Hui Yu* Quantifying Lone Pairs to Study Dative Bonds
11:00 - 11:15			
11:15 - 11:30	**6A1-5I**: *Cheol Ho Choi* MRSF-TDDFT: A Good Way of Introducing Strong Correlation	**6B1-5I**: *Hiroshi Fujisaki* Weighted ensemble simulations applied to conformational changes of proteins	**6C1-5I**: *Miho Hatanaka* Excited states of cerium photocatalysts through a machine learning lens
11:30 - 11:45			
11:45 - 12:00	**6A1-7I**: *Hiromi Nakai* Chemical Concept for Understanding the S_0/S_1 Minimum Energy Conical Intersection	**6B1-7I**: *Gerhard Hummer* Molecular simulations in the era of AI and exascale computing	**6C1-7C:** *Tao Yang* Endohedral Metal-Metal-Bonding Fullerenes
12:00 - 12:15			**6C1-8C:** *Joyata Kumar Saha* Exploring the impact of various gases on planarity and gas sensitivity of conducting polymers using DTF study
12:15 -	**Excursion**		

Thursday, September 7, 2023

8:30 -	**Registration Desk Open** (Frontier Applied Science Bldg.)		
Plenary Lecture (Large Auditorium) Chair: Hiroshi Nakatsuji			
9:00 - 9:45	**7PL-1**: *Eberhard K. U. Gross* The exact factorization, a universal approach to non-adiabaticity		
9:45 - 10:15	**Coffee Break**		
	7A1. Theory, Method, & Computation (Large Auditorium) Chair: Chaoyuan Zhu	**7B1. Biomolecule & Drug Design** (Suzuki Hall) Chair: Masataka Nagaoka	**7C1. Catalyst, Surface, & Clusters** (Seminar Room 2) Chair: Shigeyoshi Sakaki
10:15 - 10:30	**7A1-1I**: *Zhenggang Lan* Nonadiabatic Dynamics and Machine Learning	**7B1-1I**: *Dongqing Wei* AIDD and drug candidates by super-computing: Anti-Aging, Cancer and Covid-19	**7C1-1I**: *Michel Dupuis* Electronic Structure and Dynamics of Excitons and Polarons in Fe_2O_3 for Solar-to-Fuel Conversion
10:30 - 10:45			
10:45 - 11:00	**7A1-3I**: *Jian Liu* New Phase Space Formulation of Quantum Mechanics for Nonadiabatic Systems	**7B1-3I**: *Toru Shiozaki* Quantum enhanced lead optimization for small molecule drug discovery	**7C1-3C**: *Hajime Suzuki* 2 Dimensional Dodecagonal Nitride and Graphenylene via First Principle Calculations
11:00 - 11:15			**7C1-4C**: *Thanaset Kititheerakul* Mechanisms of Nickel and Palladium Catalyzed Ethylene and Carbon Monoxide Copolymerization: A Density Functional Study
11:15 - 11:30	**7A1-5I**: *Kazuo Takatsuka* Persisting multi-dimensional nonadiabatic interactions in densely quasi-degenerate excited states	**7B1-5C**: *Yuta Hori* Theoretical study for the active site in oxidized [NiFe]-hydrogenase	**7C1-5C**: *Phiphob Naweephattana* The Role of Organoaluminum and Electron Donors in the Propene Insertion on Ziegler Natta Cluster Model: A Density Functional Study
11:30 - 11:45		**7B1-6C**: *Toyokazu Ishida* Theoretical Insight into Catalytic Mechanism of GH11 Xylanase: *ab initio* QM/MM Modeling based on Neutron Structure	**7C1-6C**: *Andrey Lyalin* Role of interface effects in the catalytic activity of h-BN for oxygen reduction and hydrogen evolution reactions
11:45 - 12:00	**7A1-7C**: *Katherine N. Ferreras* Incorporating Dynamic Electron Correlation into the SF-ORMAS-CI Method via Pair-Density Functional Theory		**7C1-7C**: *Kanami Sugiyama* Reaction path search and its kinetic analysis of methanol decomposition on Pt(111) surface
12:00 - 12:15	**7A1-8C**: *Pinku Nath* Development of an automated methodology to identify key features in a dynamic of chemical reaction		**7C1-8C**: *Lauren Takahashi* Catalyst Network Method: A non-machine learning approach to designing catalysts for methane oxidation
12:15 - 13:45	**Lunch Break**		

Thursday, September 7, 2023

Plenary Lecture (Large Auditorium) Chair: Piotr Piecuch			
13:45 - 14:30	**7PL-2**: *Shuhua Li* Block-correlated coupled cluster methods for strongly correlated systems		
14:30 - 15:00	**Coffee Break**		
	7A2. Theory, Method, & Computation (Large Auditorium) Chair: Rika Kobayashi	**7B2. Chemical Reaction & Dynamics** (Suzuki Hall) Chair: David M. Leitner	**7C2. Quantum Computing** (Seminar Room 2) Chair: Debashree Ghosh
15:00 - 15:15	**7A2-1I**: *Ayako Nakata* Large-scale DFT calculations using multi-site support functions for materials with complex structures	**7B2-1I**: *Srihari Keshavamurthy* Dynamical implications of hilltops and calderas	**7C2-1I**: *Kenji Sugisaki* Development of Quantum Algorithms for Direct Calculation of Energy Gaps
15:15 - 15:30			
15:30 - 15:45	**7A2-3I**: *Yuriko Aoki* Order-N Elongation method toward multiscale calculations	**7B2-3I**: *Tamiki Komatsuzaki* A Structure of Timescale Hierarchy in Reaction Network	**7C2-3I**: *Wataru Mizukami* Approaching Quantitative Quantum Chemical Calculations with Quantum Computing
15:45 - 16:00			
16:00 - 16:15	**7A2-5I**: *Feng Long Gu* Progress on the Computational Methods based on Non-orthogonal Localized Molecular Orbitals	**7B2-5I**: *Elfi Kraka* Reaction Mechanism - Explored with the Unified Reaction Valley Approach (URVA)	**7C2-5C**: *Bruno Senjean* Toward Density Functional Theory on Quantum Computers
16:15 - 16:30			**7C2-6C**: *Hiroshi C. Watanabe* Sequential optimal selections of single-qubit gates in parameterized quantum circuits
16:30 - 16:45	**7A2-7I**: *Dmitri G. Fedorov* Molecular binding and interactions analyzed with quantum-chemical calculations	**7B2-7C**: *Takuro Tsutsumi* Analysis of Branching Reaction Dynamics based on Reduced-dimensionality Reaction Space	**7C2-7I**: *Takeshi Yanai* Analytic nuclear energy gradients of state averaged DMRG-CASSCF theory
16:45 - 17:00		**7B2-8C**: *Tatsuhiro Murakami* Machine-learning analysis and molecular dynamics for the post-transition-state bifurcation	
17:00 - 19:00	**7Po. Poster Presentation 2 (Centennial Hall, School of Medicine)**		

Friday, September 8, 2023

8:30 -	**Registration Desk Open** (Frontier Applied Science Bldg.)		
Plenary Lecture (Large Auditorium) Chair: Mark S. Gordon			
9:00 - 9:45	**8PL-1**: *Chao-Ping Hsu* Dynamic disorder of nonpolar systems: machine-learned electron transfer coupling and outer-shell reorganization energy		
9:45 - 10:15	**Coffee Break**		
	8A1. Theory, Method, & Computation (Large Auditorium) Chair: Masanori Tachikawa	**8B1. Biomolecule & Drug Design** (Suzuki Hall) Chair: Dongqing Wei	**8C1. Catalyst, Surface, & Clusters** (Seminar Room 2) Chair: De-en Jiang
10:15 - 10:30	**8A1-1I**: *Motoyuki Shiga* Brownian Chain Molecular Dynamics: A path integral approach for vibrational spectra	**8B1-1I**: *Edina Rosta* Enhanced Sampling Simulations of Biomolecular Systems	**8C1-1C**: *Ray Miyazaki* Identifying materials genes describing catalytic CO_2 hydrogenation: an AI approach with theoretical and experimental data
10:30 - 10:45			**8C1-2C**: *Shengzhou Li* Large-scale DFT and machine learning for the investigation of electronic structure: a study on supported metallic nanoparticles
10:45 - 11:00	**8A1-3I**: *Satoshi Yabushita* On the applicability of the CPKS equations without basis function derivative terms to the IR intensities of CH and OH vibrations	**8B1-3I**: *Shigehiko Hayashi* Atomistically deciphering functional activation processes of photoreceptor proteins with hybrid molecular simulations	**8C1-3C**: *Ziyun Wang* Rational Catalyst Design for CO_2 Electrochemical Reduction Reaction
11:00 - 11:15			**8C1-4C**: *Tomoko Yokaichiya* Effects of lateral interactions on surface chemical reactions revealed by kinetic Monte Carlo simulations with neural network potentials
11:15 - 11:30	**8A1-5C**: *Yasunari Zempo* Spectrum analysis with TDDFT time-series data	**8B1-5I**: *Fahmi Himo* The quantum chemical cluster approach as a tool in biocatalysis	**8C1-5I**: *Akira Nakayama* Microscopic understanding of interface at liquid/solid-oxide and molecular adsorption on the surface by neural network potentials
11:30 - 11:45	**8A1-6C**: *Nobuhiko Akino* Spectrum Analysis of Organic Materials by Real Space and Real Time TDDFT		
11:45 - 12:00	**8A1-7C**: *Shuta Fukuura* Lennard-Jones potential based particle swarm optimization: A promising alternative to density functional theory calculations for geometry optimization of host-guest nano-structures	**8B1-7C**: *Kai-Chung Lau* Gas Phase Reaction Mechanism and Energetics of CH_4 and V^+ (^5D and ^3F) ion	**8C1-7I**: *Karsten Reuter* Exploring Catalytic Reaction Networks with Machine Learning
12:00 - 12:15	**8A1-8C**: *Yang Wang* Chemical insights from quantitative resonance theory analysis of DFT wave functions		
12:15 - 13:45	**Lunch Break**		

Friday, September 8, 2023

Plenary Lecture (Large Auditorium) Chair: Kazuo Takatsuka			
13:45 - 14:30	**8PL-2**: *Nancy Makri* Real-Time Path Integral Methods for Exciton-Vibration Dynamics		
14:30 - 15:00	**Coffee Break**		
	8A2. Chemical Reaction & Dynamics (Large Auditorium) Chair: Akira Nakayama	**8B2. Machine Learning & Informatics** (Suzuki Hall) Chair: Johannes Hachmann	**8C2. Excited State & Spectroscopy** (Seminar Room 2) Chair: Masahiro Ehara
15:00 - 15:15	**8A2-1I**: *Masataka Nagaoka* A Computational Molecular Technology for Complex Reaction Systems: Red Moon Approach	**8B2-1I**: *Randy Jalem* Designing solid electrolytes for all-solid-state batteries by high-throughput first-principles calculations and informatics approaches	**8C2-1I**: *Benjamin Lasorne* Pseudo-fragmentation at *meta* -substituted phenylene nodes within conjugated dendrimers
15:15 - 15:30			
15:30 - 15:45	**8C2-3C**: *Sergio F. Sousa* Use of QM/MM Methods in Dissecting the Role Played by Different Amino Acid Residues in the Catalytic Mechanism of Plastic PET degrading Enzymes	**8B2-3I**: *De-en Jiang* Locating hydrides in copper nanoclusters by deep learning	**8C2-3I**: *Boris Le Guennic* Magnetic and (chir-)optical properties of lanthanide complexes through the prism of ab initio calculations
15:45 - 16:00	**8C2-4C**: *Yusuke Ootani* Density-Functional Tight Binding Molecular Dynamics Approach for Deformation/Fracture Mechanisms of Molecular Crystals		
16:00 - 16:15	**8C2-5C**: *Shun Yokoi* Structural and Computational Insight into Dynamics and Intermediate State in Activation of Orexin 2 Receptor	**8B2-5I**: *U. Deva Priyakumar* Molecular/Material generators: de novo design using artificial intelligence	**8C2-5I**: *M. Elena Martin* Study of the photophysical and photochemical properties of 3 hydroxyflavone in ethanol solution. Implicit vs explicit solvent models
16:15 - 16:30	**8C2-6I**: *Michelle L. Coote* (online) Catalysing reactions with electric fields		
16:30 - 16:45		**8B2-7C**: *Fernando Garcia-Escobar* Designing new Noble Metal-based Water-Gas Shift Catalysts from Literature Data	**8C2-7C**: *Masahiro Higashi* Computational analysis of excited-state properties of donor-acceptor linked molecules in condensed phases
16:45 - 17:00		**8B2-8C**: *Mikhail Tsitsvero* Prediction of NMR spectrum for dynamic molecules by machine learning: a case study of trefoil knot molecule	**8C2-8C**: *Benjamin N. Frandsen* Alien Atmospheric Chemistry and Spectroscopy involving Sulfur Compounds
18:00 - 20:00	**Banquet (Keio Plaza Hotel)**		

Saturday, September 9, 2023

8:30 -	**Registration Desk Open** (Frontier Applied Science Bldg.)		
Plenary Lecture (Large Auditorium) Chair: Fahmi Himo			
9:00 - 9:45	**9PL-1**: *Feliu Maseras* The challenge of computational homogeneous catalysis		
9:45 - 10:15	**Coffee Break**		
	9A1. Theory, Method, & Computation (Large Auditorium) Chair: Shuhua Li	**9B1. Maeda ERATO Special Session** (Suzuki Hall) Chair: Satoshi Maeda	**9C1. Condensed Phase** (Seminar Room 2) Chair: Amalendu Chandra
10:15 - 10:30	**9A1-1I**: *Takahito Nakajima* Molecular Simulations and Informatics on Fugaku	**9B1-1:** *Satoshi Maeda* Session Introduction: From the Interplay of Theory and Experiment to Chemical Reaction Design and Discovery by Combining Computation, Informatics, and Experiment	**9C1-1I**: *Hirofumi Sato* A multifaceted approach to various chemical processes in condensed phases
10:30 - 10:45		**9B1-2:** *Shigeyoshi Sakaki* How Much Can Theory Contribute to Today's Chemistry? Interplay between Theory and Experiment, and Beyond	
10:45 - 11:00	**9A1-3I**: *Roberto Cammi* Quantum Chemistry at the high pressure with the eXtreme Pressure Polarizable Continuum Model (XP-PCM)		**9C1-3I**: *Shinji Saito* Structural change dynamics in proteins and liquids
11:00 - 11:15		**9B1-4:** *Yu Harabuchi* Theoretical Chemical Reaction Database Based on Quantum Chemistry-Aided Retrosynthetic Analysis (QCaRA) Toward Chemical Reaction Discovery	
11:15 - 11:30	**9A1-5I**: *Masahiro Ehara* Photofunctions of complex systems and nanoclusters focusing on inverse design approach	**9B1-5:** *Tsuyoshi Mita* AFIR-Based Reaction Design and Realization: Three-component Reactions using Difluorocarbene and Free Radicals	**9C1-5C**: *Tamar Goldzak* Spin component scale MP2 methods for solids
11:30 - 11:45		**9B1-6:** *Satoru Iwata* Mathematical Informatics for Chemical Reactions	**9C1-6C**: *Makito Takagi* Theoretical study on excess proton/deuteron in light/heavy water solvent by using path integral molecular dynamics method
11:45 - 12:00	**9A1-7C**: *Takafumi Shiraogawa* Exploration of Chemical Space for Designing Functional Molecules Accounting for Geometric Stability		
12:00 - 12:15		**9B1-8:** *Wataru Matsuoka* Virtual Ligand Strategy in Transition Metal Catalysis Toward Computational Catalyst Design	
12:15 - 13:45	**Lunch Break**		

Saturday, September 9, 2023

	9A2. Theory, Method, & Computation (Large Auditorium) Chair: Eberhard K. U. Gross	**9B2. Machine Learning & Informatics** (Suzuki Hall) Chair: Randy Jalem	**9C2. Chemical Reaction & Dynamics** (Seminar Room 2) Chair: Yu Harabuchi
13:45 - 14:00	**9A2-1I**: *Takao Tsuneda* Reactive orbital energy theory serving the foundation for the electronic theory and revealing the driving forces of reactions	**9B2-1I**: *Rika Kobayashi* Machine Learning Interatomic Potentials in Chemistry and Materials Science	**9C2-1I**: *Kaito Takahashi* Transition metal CO interaction revisited with a twist of spin
14:00 - 14:15			
14:15 - 14:30	**9A2-3I**: *Xin Xu* Doubly hybrid functionals: From molecules to extended materials	**9B2-3I**: *Qiang Cui* Machine learning in QM/MM simulations and analysis of protein allostery	**9C2-3C**: *Seba Fuyutsuki* Clumped isotope effects during C_2H_6 recombination/dissociation reactions calculated using ab-initio and canonical transition state theory
14:30 - 14:45			
14:45 - 15:00	**9A2-5I**: *Matthias Ernzerhof* The electron-centric approach to the correlation energy	**9B2-5C**: *Bo Thomsen* Telling Hydrogen Isotopologues in Bulk Water apart using Path Integral Molecular Dynamics and Machine Learning Potentials	
15:00 - 15:15		**9B2-6C**: *Ruben Staub* Accelerating Artificial Force Induced Reaction path search with Neural Network Potentials	
15:15 - 15:30	**Coffee Break**		
Plenary Lecture (Large Auditorium) Chair: Michel Dupuis			
15:30 - 16:15	**9PL-2**: *Hiroshi Nakatsuji* Quantum chemistry with accurate solutions of the Schrodinger equation		
16:15 -	**Finale**		