Wednesday, May 18

10:00 - 11:00 Registration

Session I
Chairman: Jiří Pittner

11:00		Welcome address
11:10	Hiroshi Nakatsuji	Structure of the Exact Wave Function: Locality of the Scaling Operator
11:40	Petr Čársky	Prospects of Using Mixed Gaussian and Plane-Wave Basis Sets in Mainstream Quantum Chemistry
12:10	Jozef Noga	Orbital Optimized MBPT(2) via Non-Unitary Transformation
12:40		Lunch

Session II (Biomolecular systems)
Chairman: Zdeněk Havlas

14:00	Pavel Hobza	Non-Covalent Interactions
14:30	Shigenori Tanaka	Large-Scale Ab Initio Simulations for Biomolecular Systems
15:00	Jan Řezáč	S66 - New Benchmark Dataset for Non-Covalent Interactions
15:30	Shigeki Yamamoto	Peptide Solution Structure based on Raman Optical Activity
16:00		Coffee Break

Session III (Excited States, Molecular Properties)
Chairman: Lubomír Rulíšek

16:20	Shigeyoshi Sakaki	Theoretical Study of Dinuclear Transition Metal Complexes: Interesting Electronic Structures and Molecular Properties
16:50	Koji Ohta	Two-Photon Absorption Properties of Extended π-Conjugated Molecular Systems

17:20	Jun-ya Hasegawa	Excited States of Photo-Functional Proteins: SAC-CI Study
17:50		Young Investigator Award Lecture

18:30 – 19:30 Poster Session I

19:30 – 21:30 Welcome Reception

Thursday, May 19

Session IV (Relativistic Effects)
Chair: Hiroshi Nakatsuji

08:40	Vladimír Malkin	Fully Relativistic Calculations of NMR and EPR Parameters
09:10	Ivan Černušák	Heavy Iodine in Spotlight
09:40	Miroslav Medveď	Second-Order NLO Responses of Halogenated (Poly)Acetylene
10:10	Mojmír Kývala	Inverse Heavy-Atom Effect in Conjugated Carbenes, Silylenes, Aldehydes and Ketones
10:40		Coffee Break

Session V (Chemical Dynamics, Photodynamics)
Chair: Miroslav Urban

11:00	Hiroki Nakamura	Nonadiabatic Chemical Dynamics: From Basic Theories to Applications
11:30	Vladimír Špirko	Nonadiabatic Corrections
12:00	Petr Slavíček	Ab Initio Phtodynamics in Condensed Phase
12:30		Lunch

Session VI (Spectroscopy)
Chair: Takeshi Yanai

13:45	Masahiro Ehara	Theoretical Spectroscopy on Photo-functional Molecules with SAC-CI
14:15	Štefan Matejčík	Interpretation of Mass Spectroscopical Data Using Quantum Chemistry
14:45	Takamasa Momose	Cold and Ultracold Molecules: Current Status and Future Perspectives
15:15	Lukáš Bučinský	Relativistic Effects in Electron and Spin Densities
15:45		Coffee Break

Session VII (Solid State Chemistry, Surfaces, Functional Molecules)
Chair: Pavel Hobza

16:10	Yuriko Aoki	Development of Highly Accurate Elongation Method to Large Systems and its Application to Functional Designs
16:40	Prokopis Andrikopoulos	Examining the Role of Zeolitic Oxygens in N2O Decomposition over Fe-ferrierite
17:10	Shinji Tsuneyuki	Electronic Structure Calculation of Solids with a Similarity- Transformed Hamiltonian

17:40 – 19:00 Poster Session II

19:00 – 21:00 Conference Dinner

Friday, May 20

Session VIII (Methods, Fundamentals)
Chair: Jozef Noga

08:40	Takeshi Yanai	Advanced Multireference Method for Molecular Quantum Electronic States
09:10	Ryoichi Fukuda	Development and Applications of Direct SAC-CI Method
09:40	Hirohiko Kono	Response of Molecules to External Fields: Analysis of Time-Dependent Natural Orbitals

10:10	Ondřej Demel	Uncoupled Mukherjee's Multireference Coupled Cluster Method with Connected Triecitations
10:40		Coffee Break

Session IX (Methods, Fundamentals)
Chair: Vladimír Kellö

11:00	Mitsutaka Okumura	Theoretical investigation for Pseudo Degenerated Multi-electron Systems and Applications for Real Systems
11:30	Libor Veis	Quantum Chemistry on Quantum Computers
12:00	Robert Ponec	Splitting and/or Formation of Chemical Bonds. Insights from the Momentum Space
12:30		Lunch

Session X (Chemical Reactions)
Chair: Shigeyoshi Sakaki

13:45	Tibor András Rokob	Disulfide Activation and Carbon-Sulfur Coupling via Copper(III): Intramolecular Disproportionation of Imine Disulfides
14:15	Tetsuya Taketsugu	Extension of Ab initio Molecular Dynamics Approach to Excited-State Reactions and Tunneling Reactions
14:45	Koichi Ohno	Automated Global Reaction Route Mapping on the Potential Energy Surface
15:15		Coffee Break

Session XI (Condensed Phase, Functional Materials)
Chairs: Jiří Pittner, Lubomír Rulíšek

15:35	Ondřej Maršálek	Hydrogen Forms in Water by Proton Transfer to a Distorted Electron
16:05	Manabu Sugimoto	Computational Informatics on Chemical Patterns in Functional Molecules: Toward an Understanding, Predictions, and Design
16:35		Concluding Remarks, Departure