# Day 1: May 23 (Fri.)

12:00 Registration desk opens

12:50-13:00 Opening address (Henry F. Schaefer III)

Chair: Seiichiro Ten-no

13:00-13:30 O1-1L **Troy Van Voorhis**
*Bootstrap Embedding for Molecules and Solids*

13:30-14:00 O1-2L **Cristina Puzzarini**
*Modeling of gas-phase reactions*

14:00-14:30 Coffee break

Chair: Shuhua Li

14:30-14:50 O1-3S **Ayako Nakata**
*Large-scale DFT calculations on the site and size dependence of the electronic structure of metallic nanoclusters*

14:50-15:10 O1-4S **Tetsuya Taketsugu**
*Theoretical study of reaction path curvature and bifurcation*

15:10-15:30 Coffee break

15:30-16:00 O1-5L **Anna I. Krylov**
*Quantum chemistry in the continuum*

16:00-16:30 O1-6L **Stella Stopkowicz**
*Quantum chemical prediction for the assignment of spectra from strongly magnetized white dwarf stars*

16:30-17:00 O1-7L **T. Daniel Crawford**
*Advanced Quantum Chemical Methods for Chiroptical Spectroscopy*

17:00- Welcome Reception

# Day 2: May 24 (Sat.)

Chair: Masahiro Higashi

9:30-10:00 O2-1L **Benedetta Mennucci**
*A Quantum Chemical Perspective of the Design Principles of Light Harvesting in plants*

10:00-10:30 O2-2L **Daisuke Yokogawa**
*Development of solvation theories based on Reference Interaction Site Model Self-Consistent Field*

10:30-11:00 Coffee break

11:00-11:30 O2-3L **Stefan M. Kast**
*ML-enhanced integral equation theory for solvation free energies*

11:30-12:00 O2-4L **Akihiro Morita** (in honor of Shigeki Kato)
*Our memory of Professor Shigeki Kato*

12:00-13:30 Lunch break

Chair: Stefan M. Kast

13:30-14:00 O2-5L **Jiali Gao**
*Multistate Density Functional Theory and Applications*

14:00-14:20 O2-6S **Christopher J. Stein**
*Solvation models from a probabilistic view on the solute-solvent interaction energy*

14:20-14:50 Coffee break

Chair: Cristina Puzzarini

14:50-15:10 O2-7S **Andreas Hansen**
*Accurate calculation of non-covalent interactions for large molecules*

15:10-15:30 O2-8S **Dmitri G. Fedorov**
*Development and applications of energy decomposition analyses*

15:30-16:00 Coffee break

16:00-16:30 O2-9L **Edward Valeev**
*TBA*

16:30-17:00 O2-10L **Shuhua Li**
*Block-correlated Coupled Cluster Methods for Ground-state and Excited States of Strongly Correlated Systems*

17:00-18:20 Poster session I

# Day 3: May 25 (Sun.)

Chair: Miho Hatanaka

9:30-10:00 O3-1L **Fernanda Duarte**
*Beyond static DFT: Modelling Chemical Reactions in Solution with MLIPs*

10:00-10:30 O3-2L **Masahiro Higashi**
*QM/MM-based analysis of photophysical properties in condensed phases*

10:30-11:00 Coffee break

11:00-11:30 O3-3L **Satoshi Maeda**
*On-the-fly kinetic simulation based on automated reaction path exploration using the global reaction route mapping (GRRM) strategy*

11:30-12:00 O3-4L **Peter Pulay** (in honor of Keiji Morokuma)
*A Tribute to Keiji Morokuma*

12:00- Lunch break & free afternoon

# Day 4: May 26 (Mon.)

Chair: Yasuteru Shigeta

9:30-10:00 O4-1L **Francesco A. Evangelista**
*Multireference Unitary Electronic Structure Theories for Electronically Excited States: Classical and Quantum Approaches*

10:00-10:30 O4-2L **Wataru Mizukami**
*Practical Quantum-Classical Hybrid Algorithms Under Shot Budget Constraints*

10:30-11:00 Coffee break

11:00-11:30 O4-3L **Andreas Savin**
*A modified expression for the Hamiltonian expectation value exploiting the short-range behavior of the wave function*

11:30-12:00 O4-4L **Henryk Witek** (in honor of Kimihiko Hirao)
*Professor Kimihiko Hirao: An eminent scientist and outstanding organizer of science*

12:00-13:30 Lunch break

Chair: Martin Head-Gordon

13:30-14:00 O4-5L **Trond Saue**
*QED for molecules*

14:00-14:30 O4-6L **Julien Toulouse**
*Relativistic electronic-structure theory based on effective quantum electrodynamics*

14:30-15:00 Coffee break

Chair: Jun-ya Hasegawa

15:00-15:20 O4-7S **Luca Klaus Erhart**
*Chebyshev Approximated Variational Coupled Cluster for Quantum Computing*

15:20-15:40 O4-8S **Karl Pierce**
*Application of the Canonical Polyadic Decomposition in the Pursuit of Extremely Low-Scaling Correlation Methods*

15:40-16:00 Coffee break

16:00-16:30 O4-9L **Roland Lindh**
*The Reduced Variation Optimization Procedure: A qualitative analysis*

16:30-17:00 O4-10L **Martin Head-Gordon**
*Some recent results on developing and assessing density functionals*

17:00-18:20 Poster session II

# Day 5: May 27 (Tue.)

Chair: Masahiro Ehara

9:30-10:00 O5-1L **Dominika Zgid**
*Relativistic GW for solids and molecules*

10:00-10:30 O5-2L **Daniel Kats**
*Tensor Decomposed Distinguishable Cluster Methods*

10:30-11:00 Coffee break

11:00-11:30 O5-3L **Debashis Mukherjee**
*TBA*

11:30-12:00 O5-4L **Hiromi Nakai** (in honor of Hiroshi Nakatsuji)
*Professor Hiroshi Nakatsuji: In Pursuit of Quantum Chemical Principles*

12:00-13:30 Lunch break

13:30-14:50 Poster session III

Chair: Piotr Piecuch

14:50-15:10 O5-5S **Viktor N. Staroverov**
*Electronic energies from exact and approximate electron densities*

15:10-15:30 O5-6S **Libor Veis**
*Variational Quantum Eigensolver Boosted by Adiabatic Connection*

15:30-16:00 O5-7L **Joonhoo Lee**
*Ab-initio Auxiliary-Field Quantum Monte Carlo in the Thermodynamic Limit*

16:00-16:30 Coffee break

Chair: T. Daniel Crawford

16:30-17:00 O5-8L **Piotr Piecuch**
*$H_3^+$ formation from methyl halogens and pseudohalogens: Experiment, theory, and governing factors*

17:00-17:30 O5-9L **Yuki Kurashige**
*Tensor & Neural networks for quantum dynamics with many degree-of-freedom*

17:30-18:00 O5-10L **Gustavo Scuseria**
*Symmetry-Projected Coupled Cluster Theory*

18:00- Banquet (reservation required)

# Day 6: May 28 (Wed.)

Chair: Takeshi Yanai

9:30-10:00 O6-1L **So Hirata**
*Failures of Feynman Propagators*

10:00-10:30 O6-2L **Kimihiko Hirao**
*Long-Range-Corrected (LC) Density Functionals Examination of How Well LC Functionals Satisfy Koopmans' Theorem*

10:30-11:00 O6-3L **Hiroshi Nakatsuji**
*Exact scaled Schrödinger equation theory combined with SAC/SAC-CI theory and electrostatic force theory*

11:00- Closing