

Schedule

Tuesday, October 5th

Session 1: Two-electron Reduced Density Matrix Theory 14:00 - 15:45

(8 AM EDT - 9:45 AM EDT)

Session chair: David Mazziotti (University of Chicago)

14:00 - 14:40: **Laura Gagliardi (University of Chicago)** - Active-space based methods for strongly correlated systems

14:40 - 15:20: **Eugene DePrince (Florida State University)** - Reduced-density-matrix-based descriptions of dynamic and nondynamic electron correlation

15:20 - 15:45: **Jan-Niklas Boyn (University of Chicago)** - Variational 2-RDM method for the resolution of strongly correlated electronic structure

Flash Session: 18:00 - 19:00

(12 PM EDT - 1 PM EDT)

(brief 2 minute summaries of all contributed talks)

Session 2: Density Matrix Renormalization Group 20:00 - 22:00

(2 PM EDT - 4:00 PM EDT)

Session chair: Peter Knowles (Cardiff University)

20:00 - 20:40: **Uli Schollwöck (LMU Munich)** - Introduction to MPS

20:40 - 21:20: **Stefan Knecht (GSI Darmstadt)** - Shedding light on the chemistry of (super-)heavy elements with electronic structure theory

21:20 - 22:00: **Örs Legeza (Wigner Research Center Budapest)** - Tensor network state methods in material science and ab initio quantum chemistry

Wednesday, October 6th

Session 3: Wave Functions: Correlations and Scaling 9:00 - 10:45

(3 AM EDT - 4:45 AM EDT)

Session chair: Stefan Knecht (GSI Darmstadt)

9:00 - 9:40: **Peter Knowles (Cardiff University)** - Multiconfigurational methods for excited states

9:40 - 10:20: **Christian Ochsenfeld (LMU Munich)** - Linear-scaling methods for solving the Schrödinger equation of complex systems

10:20 - 10:45: **Tatjana Korona (University of Warsaw)** - Symmetrized systematic molecular fragmentation as a tool for exploring intermolecular interaction energy

Session 4: Density and Reduced Density Matrix Functional Theories 14:00 - 16:25

(8 AM EDT - 10:25 AM EDT)

Session chair: Christian Schilling (LMU Munich)

14:00 - 14:40: **Weitao Yang (Duke University)** - Describing strong correlation in density functional theory

14:40 - 15:20: **Hardy Gross (University of Jerusalem)** - DFT, RDMFT, and the exact electron factorization

15:20 - 16:00: **Mario Piris (Ikerbasque - Basque Foundation for Science)** - From 1RDMFT to NOF approximations

16:00 - 16:25: **Julia Liebert (LMU Munich)** - Ensemble reduced density matrix functional theory for excited states

Session 5: Greens Function, Coupled Cluster, and Pair Theories 20:00 - 22:00

(2 PM EDT - 4:00 PM EDT)

Session chair: Sabre Kais (Purdue University)

20:00 - 20:40: **Piotr Piecuch (Michigan State University)** - Approaching exact quantum chemistry by semi-stochastic and selected-CI-driven coupled-cluster computations

20:40 - 21:20: **Dominika Zgid (University of Michigan)** - Green's function embedding methods for solids

21:20 - 22:00: **Gustavo Scuseria (Rice University)** - Geminal theories for strong correlation

Thursday, October 7th

Session 6: Quantum Computing 14:00 - 15:45

(8:00 AM EDT - 9:45 AM EDT)

Session chair: Kade Head-Marsden (Harvard University)

14:00 - 14:40: **Sabre Kais (Purdue University)** - Quantum machine-learning for electronic structure calculations

14:40 - 15:20: **Prineha Narang (Harvard University)** - Quantum information and algorithms for correlated quantum matter

15:20 - 15:45: **LeeAnn Sager (University of Chicago)** - Exploration of highly-correlated systems on quantum devices

Panel Discussion: Correlated Electrons: Present and Beyond 18:00 - 18:45

(12:00 PM EDT - 12:45 PM EDT)

Session 7: Quantum Information 20:00 - 22:25

(2:00 PM EDT - 4:25 PM EDT)

Session chair: Örs Legeza (Wigner Research Center Budapest)

20:00 - 20:40: **Frank Verstraete (University of Gent)** - Constructing convex sets of local expectation values in correlated many-body systems

20:40 - 21:20: **Ignacio Cirac (Max Planck Institute for Quantum Optics Munich)** - Fermionic lattice systems with permutation symmetry

21:20 - 22:00: **Lexin Ding (LMU Munich)** - Orbital entanglement and correlation

22:00 - 22:25: **Patrik Thunström (Uppsala University)** - Electronic entanglement in strongly correlated materials