LUEST in TELLURIDE 2018

Meeting Location: Ah Haa School for the Arts
300 South Townsend Street, Telluride, CO 81435

Host: Telluride Science Research Center (TSRC)
Contact: Cindy Fusting 970-708-5069 or Mark Kozak 970-708-4426

Organizers: Gustavo E. Scuseria, Peter Pulay

Sunday June 3

18:00 Informal gathering at Phoenix Bean (next to Sheridan Bar)
Cash Bar. Dinner on your own.

Monday June 4

8:00 Breakfast at workshop site

9:00 James Shepherd : Exact electronic structure for hot electrons

9:45 Carlos Jimenez-Hoyos : Low-cost description of electron/hole transfer processes using non-orthogonal determinants

10:30 Coffee Break

11:00 Robert Izsak: Wave Function Methods for Excited States and Spectroscopic Applications

11:45 Tim Berkelbach : Coupled-cluster theory for condensed phase spectroscopy

12:30 Lunch on your own

14:30 Xiasong Li : Two-component Relativistic TDDFT and Coupled-Cluster Theory: Application to L-edge Spectroscopy

15:15 Francesco Evangelista : Applications of the driven SRG to large scale strongly correlated problems

16:00 Coffee Break

16:30 Dominika Zgid : Can Green's function methods be as accurate as wave function methods?

17:15 Troy van Voorhis : Incremental Embedding

18:00 Dinner on your own

Tuesday June 5

8:00 Breakfast at workshop site

9:00 Brenda Rubenstein : Ab Initio Finite Temperature Auxiliary Field Quantum Monte Carlo

9:45 Garnet Chan : Finite temperature coupled cluster and 2D tensor networks

10:30 Coffee Break

11:00 Eric Neuscamman : New Opportunities in Variational Excited States

11:45 Heather Kulik : Recovering exact conditions of electronic structure theory with semi-local DFT cost

12:30 Lunch on your own

14:30 Tom Henderson : Symmetry Projection and Coupled Cluster Theory

15:15 Ethan Qiu : Symmetry projected unrestricted coupled cluster

16:00 Coffee Break

16:30 Takashi Tsuchimochi : Recent progress on the development of spin-projected methods into the weakly correlated regime

17:15 Filip Pawlowski : Recent developments in coupled-cluster perturbation theory

18:30 **Group Dinner at Rustico;** Invited Speakers: Free
Others: Please sign up with Cindy : cindy@telluridescience.org

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Wednesday June 6

8:00 Breakfast at workshop site

9:00 Wenjian Liu : The Static-Dynamic-Static Framework for Strongly Correlated Electrons: iCI and SDSPT2

9:45 Mark Hoffman : Making iCI Work with Selection

10:30 Coffee Break

11:00 Sandeep Sharma : Treating weak and strong correlation using stochastic perturbation theory

11:45 Piotr Piecuch : High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions

12:30 Lunch on your own

14:30 Gustavo Scuseria : Hierarchical Coupled Cluster Theory

15:15 Seiichiro Ten-no : Adaptive many-body approaches

16:00 Coffee Break

16:30 Janus Eriksen : Many-Body Expanded Full Configuration Interaction

17:15 Shuhua Li : Electronic structure methods for strongly correlated systems with large active spaces

18:30 – 20:30 Picnic at Ah Haa & Poster Session (see list at the end)

Thursday June 7

8:00 Breakfast at workshop site

9:00 Mihaly Kallay : Reduced-cost correlation methods for excited states of large molecules

9:45 Jing Kong : Computation of Strong Nondynamic Correlation with DFT

10:30 Coffee Break

11:00 Ed Valeyev : Improved rank-reduced encoding of dynamical electron correlation in ground and excited states

11:45 Peter Pulay : Reference wavefunctions for strong electron correlation

12:30 Lunch on your own followed by self-organized hike

Posters

Dmytro Bykov : Unrestricted CC Methods within Divide-Expand-Consolidate Scheme

Guo Chen : Low-scaling algorithms for the approximate exchange kernel method

Dhabih Chuhai : Machine learning for quantum electron correlation

Joonho Lee : Exact Bond-Breaking with Coupled-Cluster Valence Bond Theory

Run Li : Development of Complex v2RDM Driven Relativistic CASSCF Methods

Dmytro Liakh : Fast adaptive coupled-cluster theory via hierarchical compressed tensor representations

Fang Liu : Understanding and correcting density delocalization errors in approximate DFT for transition metal chemistry

Peter Nagy : Approaching the basis set limit of CCSD(T) energies for large molecules with local natural orbital coupled-cluster methods

Minh Popis : Study of Electron-Hole Pairs by Green's Function based MCSCF

Sylvester Popis : Parallelization of ERI Recursive Functions using OpenMP

Alexander Rusakov : Green's function embedding methods for realistic solids

Avijit Shee : Coupled Cluster Green's Function using the Lanczos Algorithm and its Application to Hubbard Models

Zsuzsanna Toth : Geminal perturbation theory based on the unrestricted Hartree–Fock wavefunction

Lan Nguyen Tran : ab initio Self-energy Embedding Theory

Konstantinos Vogiatzis : Application of Quantum Chemistry and Machine Learning for Solving Complex Problems

Alicia Welden: Finite-temperature electronic structure methods from the Green's function

Alec White : A time-dependent formulation of coupled cluster for fermionic systems at finite temperature

Yanbing Zhou : Numerical Interpolation Algorithm for Matsubara Green's functions in Periodic System