LUEST in TELLURIDE 2016

Meeting Location: Wilkinson Library, 100 W. Pacific Ave
Breakfast & Posters: Arroyo Wine Bar, 220 E. Colorado Avenue

Host: Telluride Science Research Center (TSRC), http://www.telluridescience.org
Contact: Kristen Redd, TSRC Managing Director, Cell: 970-708-0827,
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Organizers: Gustavo E. Scuseria, Peter Pulay

Tuesday May 31:

17:00-19:00 Welcome reception at Arroyo Wine Bar, 220 E. Colorado Ave. **Cash Bar**.
19:00 Dinner on your own.

Wednesday June 1

7:30-9:00 Breakfast at Arroyo

9:00 Troy van Voorhis
The many-particle expansion: A systematic method for including strong correlation in DFT

9:45 Ken Jordan
Muticonfigurational Trial Functions in Quantum Monte Carlo Calculations

10:30 Coffee Break

11:00 Dominika Zgid
Green's function embedding methods for molecules and solids

11:45 Carlos Jimenez-Hoyos
Embedding methods in the presence of strong correlation

12:30 Lunch on your own

14:30 Roi Baer
Stochastic GF2 and GW calculations for large systems

15:15 Miguel Morales
QMC Benchmark of Exchange-Correlation Functionals for Liquid Water

16:00 Coffee Break

16:30 Sandeep Sharma
Treating large active and virtual spaces using DMRG and FCIQMC

17:15 Seiichiro Ten-no
Advances in model space quantum Monte Carlo

18:00 Dinner on your own

19:30 - 21:30 Poster Session #1 Posters 1-12 Beer & Wine

Arindam Chakraborty	Describing electronic excitations in atoms, molecules, and clusters using eh-mcCC
Franco Egidi	Electronic Structure Methods for Relativistic Effects in Excited States
Matthew Hermes	Nature of the many-body similarity transformed coupled cluster Hamiltonian
Kevin Gasperich	Diffusion Monte Carlo calculations on systems with degeneracies and near degeneracies
Joshua Goings	Recent advances in real-time TDDFT for the description of optical activity
John Gomez	Singlet paired coupled cluster theory for open-shells
Marco Govoni	Computing quasiparticle energies for large systems Without Empty STates (WEST)
Gerald Knizia	Simple quantum embedding for active regions of realistic molecules
Wei Li	Fragmentation based quantum chemistry approach for large systems
Zhendong Li	Low-rank tensor approximations for many-electron wave functions in Hilbert space
Elvira Sayfutyarova	Spin-orbit coupling with the spin-adapted density matrix renormalization group
Vamsee Vora	Orbital Optimized Random Phase Approximation

Thursday June 2

7:30-9:00 Breakfast at Arroyo

9:00 Eric Neuscamman
Exciting developments in variational Monte Carlo

9:45 So Hirata
Brueckner-Goldstone quantum Monte Carlo

10:30 Coffee Break

11:00 Shuhua Li
Generalized energy-based fragmentation approach for structures and spectra of molecules in condensed phases

11:45 George Booth
A novel combination of variational and projector QMC for polynomial strong correlation

12:30 Lunch on your own

14:30 Peter Pulay
Finding symmetry-breaking solutions of the SCF equations: The case of triplet instability

15:15 Takashi Tsuchimochi
Effective multi-reference configuration interaction from spin-projected HF

16:00 Coffee Break

16:30 Lucas Wagner
Progress towards a consistent and testable link between effective models and correlated ab initio calculations

17:15 Gustavo Scuseria
New vistas on strong correlation from symmetry projection

19:00 Group Dinner at Rustico (114 E. Colorado Ave). **Free for invited speakers. Others are welcome:** subsidized at $40 per person (including wine); please sign up.

Friday June 3

7:30-9:00 Breakfast at Arroyo

9:00 Frank Neese
New developments in domain based pair natural orbital correlation methods

9:45 Piotr Piecuch
SR CC and EOM CC Methods for Multi-Reference Problems

10:30 Coffee Break

11:00 Xiasong Li
Linear Response and Real-Time Two-Component Relativistic Electronic Structure Methods

11:45 Laura Gagliardi
Multiconfiguration Pair-Density Functional Theory

12:30 Ali Alavi
Stochastic approach to large-scale CASSCF and MR perturbation theory

13:15 Free Afternoon

20:00 - 22:00 Poster Session #2 Posters 13-23 Beer & Wine

Matthias Degroote	Polynomial Similarity Transform for strong correlation
Adam Holmes	Efficient Heat-bath Sampling in Fock Space
Chad Hoyer	Multiconfiguration Pair-Density Functional Theory for Excited-State Chemistry
Jing Ma	Exploring Low-lying Singlet Excited States of Molecular Clusters

John Mintmire	Truncation Algorithms for One-Dimensional Lattice Sums of Coulomb Integrals
Zhigang Ni	Quasiatomic Orbitals for Pipek-Mezey Localization and Molecular Properties
Tuguldur Odbadrakh	Course graining dispersion interactions using quantum Drude oscillators
Alexander Sokolov	Time-dependent perturbation theory for multi-reference problems
Zsuzsanna Toth	Revisiting Hartree-Fock instability: energy surfaces
Yiheng Qiu	Symmetry projection as an extended coupled cluster theory
Martin Zonda	Perturbation theory of a quantum dot attached to superconducting leads

Saturday June 4

7:30-9:00 Breakfast at Arroyo

9:00 Christine Isborn
Size-Dependent Errors in DFT in Vacuum and Solution

9:45 Angela Wilson
Theoretical approaches for transition metals and heavy elements

10:30 Coffee Break

11:00 Emanuel Gull
Solutions of the Two Dimensional Hubbard Model: Benchmarks and Results from a Wide Range of Numerical Algorithms

11:45 Johannes Dieterich
New developments in reduced scaling wavefunction and linear-scaling density functional theories

12:30 Lunch on your own

14:30 Marcel Nooijen
Coupled Cluster Theory for Magnetic Systems

15:15 Toru Shiozaki
Predicting magnetic properties of strongly correlated systems

16:00 Coffee Break

16:30 Francesco Evangelista
New methods for strongly correlated electrons with tunable accuracy

17:15 Garnet Chan
Periodic quantum chemistry

18:00 Dinner on your own

Sunday June 5: Departure