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,
         Office: 970-729-8375, kristen@telluridescience.org
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