LUEST in TELLURIDE 2012

Meeting Location

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

Meeting Host

Telluride Science Research Center (TSRC)
Contact: Nana Naisbitt 970-708-0004 or Jake Sullivan 970-708-7447

Meeting Organizers

Gustavo E. Scuseria
Peter Pulay

Sunday June 17:

5:00 - 7:00 pm Check-in at the Ah Haa School for the Arts

Monday June 18

7:30 Check-in and coffee (Ah Haa School for the Arts)

8:00 Breakfast at workshop site (Ah Haa School for the Arts)

9:00 **Ali Alavi**, University of Cambridge
Recent progress with FCIQMC: methods and applications

9:45 **Cyrus Umrigar**, Cornell University
Semistochastic Quantum Monte Carlo -- How to have most of your cake and eat all of it

10:30 **Coffee Break**

11:00 **Seiichiro Ten-no**, Kobe University
F12 theory in conjunction with relativity and determinantal-based QMC method

11:45 **Hiroshi Nakatsuji**, Quantum Chemistry Research Institute
Topics on solving the Schrődinger equation

12:30 Lunch on your own

14:00 **Martin Head-Gordon**, University of California, Berkeley
GVB and CC: a marriage of two wonderful theories

14:45 **Yuki Kurashige**, Institute for Molecular Science
Electronic-structure of Mn_4Ca cluster in photosystem II: Insights from quantum-chemical density-matrix renormalization group theory

15:30 Coffee Break

16:00 **Markus Reiher**, ETH Zurich
Tensor decompositions, entanglement, and other unconventional approaches to challenging problems in transition metal chemistry

16:45 **Gustavo Scuseria**, Rice University
Symmetry Breaking and Restoration

17:30 Discussion

18:00 Dinner on your own

19:30 - 21:30 **Poster Session #1** Cash Bar

Tuesday June 19

8:00 Breakfast at workshop site

9:00 **Filipp Furche**, University of California, Irvine
Making DFT accurate: Molecular properties within the random phase approximation

9:45 **Kasia Pernal**, Technical University of Lodz
Extended random phase approximation with reconstructed second-order density matrix applied to computing excitation energies

10:30 Coffee Break

11:00 **Andreas Savin**, CNRS and UPMC Paris Sorbonne
Combining DFT and wave function methods

11:45 **Giulia Galli**, University of California, Davis
Improving accuracy and efficiency of first principle calculations of excited state properties: many body perturbation theory without empty states

12:30 Lunch on your own

14:00 **Paola Gori-Giorgi**, Free University Amsterdam
The strong-interaction limit of DFT: Recent developments

14:45 **Francois Gygi**, University of California, Davis
Acceleration of hybrid DFT simulations using recursive subspace bisection

15:30 Coffee Break

16:00 **Tamar Stein**, Fritz Haber Center for Molecular Dynamics
Orbital Energies From Density Functional Theory

16:45 **Troy Van Voorhis**, MIT
Toward Static and Dynamic Correlation with DFT

17:30 Discussion

19:00 **Group Dinner**
La Marmotte Restaurant
150 West San Juan Avenue
Telluride, CO 81435

Wednesday June 20

8:00 Breakfast at workshop site

9:00 Bear Creek Trail Hike

14:00 **Garnet Chan**, Princeton University
Density Matrix Embedding

14:45 **Fred Manby**, University of Bristol
Capturing many-body effects through embedding

15:30 Coffee Break

16:00 **Thomas Miller**, Caltech
Embedded density functional theory methods for condensed phase reactions

16:45 **Kenneth Jordan**, University of Pittsburgh
Challenges in treating non-valence correlation bound anions of water clusters and fullerenes

17:30 Discussion

18:00 Dinner on your own

19:30 - 21:30 **Poster Session #2** Cash Bar

Thursday June 21

8:00 Breakfast at workshop site

9:00 **Shuhua Li**, Nanjing University
Cluster-in-molecule local correlation approach: Recent developments and applications

9:45 **Marcel Nooijen**, University of Waterloo
Multireference equation of motion coupled cluster theory

10:30 Coffee Break

11:00 **Martin Schuetz**, University of Regensburg
Local Coupled Cluster or else…

11:45 **Hans-Joachim Werner**, Institute for Theoretical Chemistry, University of ??
Towards scalable local coupled-cluster methods

12:30 Lunch on your own

14:00 **Robert Harrison**, Oak Ridge
Multiresolution methods for static and time-dependent electronic structure

14:45 **Eric Neuscamman**, UC Berkeley
An exactly size consistent geminal power via Jastrow factor networks

15:30 Coffee Break

16:00 **Edward Valeev**, Virginia Tech
Electron correlation via adaptive multiresolution representation: recent progress

16:45 **Joost VandeVondele**, ETH Zurich
Low scaling methods in the condensed phase: GGAs, hybrids and beyond.

17:30 Discussion

18:00 **"Picnic" dinner hosted by TSRC at the Ah Haa School of Arts**
Family members and guests welcome, free of charge

Friday June 22

8:00 Breakfast at workshop site

9:00 **Xiaosong Li**, University of Washington
Efficient first-principles solvated electronic dynamics

9:45 **Dage Sundholm**, University of Helsinki
A divide a conquer numerical approach to all-electron electronic structure calculations

10:30 **James Shepherd**, University of Cambridge
A full configuration interaction perspective on the homogeneous electron gas

11:15 Workshop End