LUEST in TELLURIDE 2014

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

Host: Telluride Science Research Center (TSRC)
Contact: Nana Naisbitt 970-708-0004 or Rory Sullivan 970-708-4542

Organizers: Gustavo E. Scuseria, Peter Pulay

Sunday June 1:

15:30 Check-in at the Ah Haa School for the Arts (coffee, tea, snacks served)

16:30 Filipp Furche
Random phase approximation renormalized many-body perturbation theory

17:15 Kizasi Yamaguchi
Developments of Broken-Symmetry Methods in Chemistry and Chemical Biology-Application to Oxygen Evolving Complex (OEC) of Photosystem II (PSII)

18:00 Dinner on your own

19:30 Welcome get-together at Arroyo Wine Bar at 220 E. Colorado Avenue
Cash Bar… Wine Specials

Monday June 2

8:00 Breakfast at workshop site

9:00 Janos Angyan
Some yet unexplored ways of using range-separated RPA for energy

9:45 Peter Pulay
Black box methods for strongly correlated systems

10:30 Coffee Break

11:00 Helen van Aggelen
Exchange-correlation energy, excitation and ionization from linear response in DFT

11:45 Weitao Yang
Particle-particle Random Phase Approximation

12:30 Lunch on your own

14:30 Fred Manby
Distinguishable clusters in coupled cluster theory

15:15 Gustavo Scuseria
Unconventional Electronic Structure Techniques

16:00 Coffee Break

16:30 Marcel Nooijen
Transform & Diagonalize approaches to electronic spectra for multireference systems

17:15 Toru Shiozaki
Diabatic model Hamiltonians from active space decomposition

18:00 Dinner on your own

19:30 - 21:30 Poster Session #1 Posters 1-10 Cash Bar

1	Irek Bulik	Density Embedding Theory for realistic Hamiltonians
2	Jason Goodpaster	Accurate and systematically improvable quantum embedding methods for complex systems
3	Dmitry Lyakh	Scale-adaptive tensor algebra for local many-body methods
4	Carlos Jimenez-Hoyos	A symmetry projected approach applied to spin lattices
5	Paul Johnson	Modelling Strong Correlation with Non-orthogonal Geminals
6	Ward Poelmans	Variational Optimization of the 2DM using GPGPU
7	Qiming Sun	Using density matrix embedding theory to construct exact QM/MM boundaries
8	Agnes Szabados	Lower bound approximations via Lowdin's bracketing function
9	Brecht Verstichel	Auxiliary field quantum monte carlo using tensor network states
10	Bo-Xiao Zheng	Towards first-principle description of high-T_c superconductors

Tuesday June 3

8:00 Breakfast at workshop site

9:00 Paul Ayers
Computationally Efficient Geminal Product Wavefunctions, and Other Wavefunction Forms Inspired by Exactly Solvable Model Hamiltonians

9:45 So Hirata
A few potentially controversial issues in many-body theory

10:30 Coffee Break

11:00 Viktor Staroverov
Explicit connections between density-functional and wavefunction methods

11:45 Peter Surjan
Generalized Distributions to Describe Quasiclassical Mechanics

12:30 Lunch on your own

14:30 Andreas Gruneis
Explicitly correlated methods for periodic systems

15:15 Georg Kresse
Low complexity RPA calculations: cubic system size scaling

16:00 Coffee Break

16:30 Beate Paulus
The method of increments applied to the metal-insulator transition in beryllium chains

17:15 Garnet Chan
Limits of accuracy in molecules and the condensed phase

18:00 Attendees not coming to Banquet: Dinner on your own

18:30 Invited & Contributed Speakers Banquet at Rustico (114 E Colorado Ave, 970-728-4046). **Others:** $55 per person ($75 with wine). Sign up and pay to Nana.

Wednesday June 4

8:00 Breakfast at workshop site

9:00 Claudia Filippi
Embedded wavefunction calculations of excited states:
Which wave functions? Which embedding?

9:45 Seiichiro Ten-no
F12 and QMC calculations on massively parallel architectures

10:30 Coffee Break

11:00 Dominika Zgid
How to make DMFT quantitative for realistic systems?

11:45 Lunch on your own

13:00 Hike

18:00 Picnic at Ah Haa

18:30 - 20:30 Poster Session #2 Posters 11-22

11	Arindam Chakraborty	Investigation of electron-hole interaction in nanoparticles using explicitly correlated wave function based methods
12	Guo Chen	Cubic Scaling Random Phase Approximation
13	Matthias Degroote	Transfer Matrices and Excitations in Tensor Network States
14	Lukas Hammerschmidt	Electron Correlation in Metal Fluorides: From Bulk to Surfaces
15	Weifeng Hu	Analytic energy gradients for quantum chemistry Density Matrix Renormalization Group
16	Daniel Lambrecht	First-principles simulation of catalyst-support interactions on amorphous silica
17	Dario Rocca	Random-phase approximation correlation energies from Lanczos chains and an optimal basis set: Theory and applications to the benzene dimer
18	Alexander Rusakov	Recovering non-local Coulomb interactions in embedding methods: from model to realistic systems
19	Sebastian Wouters	DMRG-SCF study of the singlet, triplet, and quintet states of oxo-Mn(Salen)
20	Jordan Phillips	How well can self-consistent second-order Green's function theory recover strong correlation?
21	Peter Pulay	Mixed Gaussian and Plane Wave Basis Sets
22	Alexei Kananenka	Development of DCA+GF2+DMFT multi-scale translationally invariant embedding scheme

Thursday June 5

8:00 Breakfast at workshop site

9:00 Sandeep Sharma
Realizing the spectroscopy of iron-sulfur clusters directly from entangled many-particle quantum mechanics

9:30 James Shepherd
Modern Coupled Cluster Theory for the Uniform Electron Gas

10:00 Ken Jordan
Application of multiconfigurational trial functions in QMC studies of diradical systems

10:30 Coffee break

11:00 Stijn de Baerdemacker
Integrable Richardson-Gaudin bases for Doubly-Occupied Configuration Interaction Hamiltonians

11:30 Tom Henderson
BCS Quasiparticle coupled-cluster theory

12:00 Adjourn