Virtual LUEST 2020

**Dates**: June 1–5, 8–9

**Time**: 10:30 am – 2:30 pm (EST)

**Host**: Telluride Science Research Center (TSRC),

http://www.telluridescience.org

**Contact**: Cindy Fusting, TSRC Managing Director, [cindy@telluridescience.org](mailto:cindy@telluridescience.org)

Dominika Zgid: [dominika.zgid@gmail.com](mailto:dominika.zgid@gmail.com)

Francesco Evangelista: [francesco.evangelista@emory.edu](mailto:francesco.evangelista@emory.edu)

**Organizers**: Gustavo E. Scuseria, Peter Pulay, Dominika Zgid, Francesco A. Evangelista

Direct Zoom Link: [LUEST 2020](https://zoom.us/j/95547699627?pwd=dzlEaGw3ZjRIZXA4Um1LNTlRbjUyZz09)

### Meeting schedule (all times are Eastern Standard Time)

**Monday, June 1**

10:30 **Laura Gagliardi**

Localized Active Space Self-Consistent Field

11:15 **Tim Berkelbach**

Excitons in solids from periodic CC

12:00 **Break**

1:00 **Gerald Knizia**

TBD

1:45 **Xiasong Li**

Relativistic MRCI with Tunable Correlation Space: Lessons Learned in Heavy-Element Chemistry

**Tuesday, June 2**

11:15 **Philip Shushkov**

Coupled cluster methods for quantum dynamics of closed and open systems at finite temperature

12:00 **Break**

1:00 **Tamar Stein**

1:45 **Benjamin Levine**

Electronic Structure for Nonadiabatic Dynamics

**Wednesday, June 3**

10:30 **Piotr Piecuch**

High-Accuracy Electronic Energetics by Stochastic and Deterministic Wave Function Sampling and Coupled-Cluster Computations

11:15 **Brenda Rubenstein**

Unveiling the Finite Temperature Physics of Hydrogen Chains via Auxiliary Field Quantum Monte Carlo

12:00 **Break**

1:00 **Sandeep Sharma**

Geometry optimization and dynamical correlation in transition metal systems

**Thursday, June 4**

10:30 **Kasia Pernal**

Dynamic correlation for multireference wavefunctions from adiabatic connection

11:15 **Carlos Jimenez-Hoyos**

TBD

1:00 **Eugene DePrince**

Reduced-density-matrix-based descriptions of dynamic and nondynamic electron correlation

1:45 **Alexander Sokolov**

Recent developments in algebraic diagrammatic construction theory

**Friday, June 5**

10:30 **Ed Valeyev**

Reduced-complexity representations for the wave operator: real space and LCAO

11:15 **Peter Pulay**

TBD

12:00 **Break**

1:00 **Gustavo Scuseria**

Electronic structure methods for strong correlation

1:45 **Eric Neuscamman**

New Developments in Excited-State-Specific Quantum Chemistry

**Monday, June 8**

10:30 **Takashi Tsuchimochi**

Recovering spin symmetry in classical and quantum computers

11:15 **James D. Whitfield**

TBD

12:00 **Break**

1:00 **Tom Henderson**

Post-AGP Correlated Methods

1:45 **Francesco Evangelista**

Quantum algorithms for strongly correlated electrons?

**Tuesday, June 9**

10:30 **Andreas Gruneis**

TBD

11:15 **Dominika Zgid**

Embedding methods for solids (NiO, SrVO3, MnO)

12:00 **Break**

1:00 **Heather Kulik**

Diagnosing strong correlation with machine learning

1:45 **Garnet Chan**

TBD