

New Developments in Coupled-Cluster Theory, July 29 – August 2, 2024

Location: Telluride Intermediate School, 721 W Colorado Ave, Telluride, CO 81435, USA

Organizers:

Prof. Thomas Jagau, Department of Chemistry, KU Leuven, Belgium

Prof. Anna Krylov, Department of Chemistry, University of Southern California, USA

Prof. Stella Stopkowicz, Department of Chemistry, Saarland University, Germany

TSRC Hosts:

Mark Kozak, Executive Director

Cindy Fusting, Managing Director

Sara Friedberg, Lodging & Operations Manager

Annie Carlson, Director of Donor Relations

<https://meetings.telluridescience.org/meetings/workshop-details?wid=1119>

The focus of the workshop is to facilitate in-depth discussion of current trends in coupled-cluster theory, with the emphasis on the following topics:

- strong correlation and multireference CC theory;
- unitary CC theory
- electronically excited states and open-shell species;
- large molecules and complex environments;
- relativistic CC treatments;
- algorithmic issues;
- connections with other approaches to the many-body problem;
- CC methods beyond electronic structure (nuclear structure, etc);
- extensions of CC theory driven by experiments (properties, spectroscopy modeling, etc)
- CC and machine learning

All talks are 30 min + 15 min discussion

PROGRAM

Sunday, July 28:

5:00 pm – 6:30 pm **All-Telluride Science Meet and Greet**, Alibi, 157 S Fir Street

Monday, July 29:

7:30 BREAKFAST

SESSION I (Chair: Thomas Jagau)

8:00 am Opening remarks

8:15 am Jürgen Gauss (Mainz): *A connected formulation of equation-of-motion coupled-cluster response theory*

9:00 am Daniel Crawford (Virginia Tech): *Real-time and frequency-dependent coupled cluster response theory, including beyond-Born-Oppenheimer effects*

9:45 am BREAK

SESSION II (Chair: Daniel Crawford)

10:15 am Andreas Köhn (Stuttgart): *Electronic excited states from multireference coupled-cluster response theory and its relatives*

11:00 am Pierre-Francois Loos (Toulouse): *State-specific coupled-cluster methods for excited states*

11:45 am END

SESSION III (Chair: Andreas Köhn)

6:00 pm Filippo Lipparini (Pisa): *Towards coupled cluster calculations for large symmetric molecules using Cholesky decomposition*

6:45 pm Peter Nagy (TU Budapest): *Development of an efficient local natural orbital CCSD(T) method and its application for complicated molecular interactions and reactions*

7:30 pm END

Tuesday, July 30:

7:30 am BREAKFAST

SESSION IV (Chair: Henrik Koch)

2:00 pm Stella Stopkowicz (Saarland): *Recent developments in finite-field coupled-cluster methods*

2:45 pm Petros Kitsaras (Saarland): *Geometry optimizations for ground and excited states using finite magnetic field coupled-cluster theory*

3:30 pm BREAK

SESSION V (Chair: Pierre-Francois Loos)

4:00 pm Thomas Jagau (Leuven): *Treatment of non-radiative decay processes using complex-scaled coupled-cluster theory*

4:45 pm Sarai Folkestad (Trondheim): *Entanglement coupled cluster theory for doublet systems using automatic code generation*

5:30 pm BREAK

6:30 pm – 7:30 pm **Telluride Science Town Talk by Richard Lowenberg: The Nature of Information**, Telluride Conference Center in Mountain Village, Cash Bar, Doors Open at 6:00 pm

Wednesday, July 31:

7:30 am BREAKFAST

SESSION VI (Chair: Anna Krylov)

2:30 pm Thomas Bondo Pedersen (Oslo): *Attosecond quantum dynamics with coupled-cluster theory*

3:15 pm Eirik Kjørstad (Caltech): *Unexpected hydrogen dissociation in thymine: predictions from excited state dynamics with coupled cluster theory*

4:00 pm Maristella Alessio (Leuven): *Applications of coupled-cluster theory to complex and extended open-shell systems*

4:45 pm GROUP PICTURE

5:30 pm – 7:30 pm **All Telluride Science Picnic**, free BBQ, beer, wine, and non-alcoholic beverages. Friends and family are invited free of charge, Tent behind the Intermediate School

Thursday, August 1:

7:30 am BREAKFAST

SESSION VII (Chair: Kasia Boguslawski)

1:30 pm Andreas Grüneis (TU Wien): *Understanding shortcomings of perturbative coupled-cluster theory for metals and large molecules*

2:15 pm Verena Neufeld (Caltech): *Beyond coupled cluster singles and doubles in metallic solids*

3:00 pm BREAK

SESSION VIII (Chair: Andreas Grüneis)

3:30 pm Eugene DePrince (Florida State): *Relativistic equation-of-motion coupled-cluster for single and double ionization*

4:15 pm Andre Gomes (Lille): *Explorations of molecular (response) properties for heavy element systems*

5:00 pm BREAK

SESSION IX (Chair: Mihaly Kallay)

5:30 pm Henrik Koch (SNS Pisa): *Recent advances in multi-component coupled cluster methods*

6:15 pm Kasia Boguslawski (Torun): *Elucidating chemical processes with pCCD-based methods*

7:00 pm END

Friday, August 2:

7:30 am BREAKFAST

SESSION X (Chair: Jürgen Gauss)

8:00 am Mihaly Kallay (TU Budapest): *Basis-set limit CCSD(T) energies for large molecules with local natural orbitals and reduced-scaling basis-set corrections*

8:45 am Devin Matthews (Southern Methodist): *New Developments in THC-CC*

9:30 am BREAK

SESSION XI (Chair: Stella Stopkowicz)

10:00 am Piotr Piecuch (Michigan State): *Converging high-level coupled-cluster energetics via semi stochastic, selected-CI-driven, and adaptive CC(P;Q) approaches*

10:45 am Anna Krylov (Southern California): TBA

11:30 am Closing Remarks

12:00 noon END