

Title: “New Developments in Coupled-Cluster Theory”

Organizers:

Prof. Anna Krylov, Department of Chemistry, University of Southern California, Los Angeles, USA
Prof. Jürgen Gauss, Institute of Physical Chemistry, University of Mainz, Mainz, Germany
Dr. Thomas Jagau, Department of Chemistry, University of Munich, Munich, Germany
Dr. Stella Stopkowicz, Institute of Physical Chemistry, University of Mainz, Mainz, Germany

Location: Telluride Intermediate School, 717 West Colorado Avenue, Telluride, CO 81435

TSRC Hosts: Mark Kozak (970) 708-4426, Kristen Redd (970) 708-0827

Time: July 31- August 4, 2017

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;
- electronically excited states and open-shell species;
- large molecules and complex environments;
- relativistic CC treatments;
- algorithmic issues;
- extensions of CC theory driven by experiments (properties, spectroscopy modeling, etc)

Schedule: All talks are 30 min + 15 min discussion

Sunday, July 30: 6:00-9:00 pm

***WELCOME RECEPTION AT THE PHOENIX BEAN* CASH BAR**

The Phoenix bean is located at [221 W. Colorado Ave Main Street](#). This is a newly renovated favorite of TSRC participants. They are opening their coffee shop/ bar to scientists on Sunday nights with drink specials from 6:00-9:00pm.

A representative from TSRC will be there 6-8pm to hand out badges, welcome folks to town, and answer your questions. You will need your badge for the drink specials. Guests and family members are welcome.

Monday, July 31:

7:30 BREAKFAST

MORNING SESSION (Chair: Jürgen Gauss)

8:00 Opening remarks

8:15 Frank Neese (MPI CEC) “Recent developments in local coupled cluster theory”

9:00 Evgeny Epifanovsky (Q-Chem) “Libtensor: case study in implementing and using coupled cluster theory in software”

9:45 BREAK

10:15 Henrik Koch (NTNU) “Multi-level Hartree-Fock and coupled cluster theory”

11:00 Mihály Kállay (Budapest) “Redundancy-free fragmentation-based local coupled-cluster approaches”

11:45 END

EVENING SESSION (Chair: Mihály Kállay)

7:00 Alex Thom (Cambridge) "Developments in stochastic coupled cluster theory"

7:45 Dominika Zgid (Michigan) "Green's function embedding methods and their relationship to CC"

8:30 END

Tuesday, August 1:

7:30 BREAKFAST

AFTERNOON SESSION (Chair: Frank Neese)

2:00 Thomas B. Pedersen (Oslo) "Local coupled-cluster theory with periodic boundary conditions"

2:45 Andreas Grüneis (MPI FKF) "Towards efficient periodic coupled cluster theory calculations of solids and surfaces"

3:30 BREAK

4:00 Marcel Nooijen (Waterloo) "Coupled cluster theory for periodic systems"

4:45 END

6:00-7:00 Town talk

Wednesday, August 2:

7:30 BREAKFAST

AFTERNOON SESSION (Chair: Ksenia Bravaya)

2:00 Devin Matthews (Texas) "Simple spin-adaptation for equation-of-motion coupled-cluster theory"

2:45 Stella Stopkowicz (Mainz) "Ground and excited states in strong magnetic fields with CC and EOM-CC theory"

3:30 BREAK

4:00 Andreas Köhn (Stuttgart) "Quo vadis icMRCC?"

4:45 Alexander Sokolov (CalTech) "Towards robust multi-reference coupled cluster theory: can we learn anything from perturbation theory?"

5:30 **Workshop group picture**

6:00-9:00 TSRC picknick

Thursday, August 3:

7:30 BREAKFAST

AFTERNOON SESSION (Chair: Thomas Jagau)

2:00 Anna Krylov (USC) "Non-adiabatic couplings in EOM-CC framework"

2:45 Eirik Kjørstad (NTNU) "Same-symmetry conical intersections with coupled cluster theory"

3:30 BREAK

4:00 Kaushik Nanda (USC) "New theoretical tools for analyzing two-photon absorption cross-sections"

4:45 Sonia Coriani (DTU) “Coupled cluster beamlines for modern experiments”
5:30 END

EVENING SESSION (Chair: Stella Stopkowicz)

7:00 Thomas Jagau (Munich) “Equation-of-motion coupled-cluster methods for shape and Feshbach resonances”

7:45 Ksenia Bravaya (Boston U) “Approximate EOM-CCSD models for metastable electronic states”

8:30 END

Friday, August 4:

7:30 BREAKFAST

MORNING SESSION (Chair: Anna Krylov)

8:00 Jürgen Gauss (Mainz) “Beyond standard coupled-cluster theory and towards full configuration interaction”

8:45 David Tew (Bristol) TBA

9:30 BREAK

10:00 Lan Cheng (John Hopkins) “Spin-orbit coupled cluster methods using atomic mean-field spin-orbit integrals: pilot implementation and molecular applications”

10:45 John Stanton (Florida) “Some experiments with old ideas”

11:30 Simen Kvaal (Oslo) “The bivariational principle: a rigorous Rayleigh–Ritz-like principle with applications to coupled-cluster theory”

12:15 Closing remarks and farewell, discussion about future workshops
END

Registered participants (24 total):

Ksenia Bravaya (Boston U) kbravaya@gmail.com “Approximate EOM-CCSD models for metastable electronic states”

Lan Cheng (John Hopkins) chenglanster@gmail.com “Spin-orbit coupled cluster methods using atomic mean-field spin-orbit integrals: pilot implementation and molecular applications”

Sonia Coriani (DTU) soco@kemi.dtu.dk “Coupled cluster beamlines for modern experiments”

Evgeny Epifanovsky (Q-Chem) epif@q-chem.com “Libtensol: case study in implementing and using coupled cluster theory in software”

Jürgen Gauss (Mainz) gauss@uni-mainz.de “Beyond standard coupled-cluster theory and towards full configuration interaction”

Andreas Grüneis (MPI FKF) a.grueneis@fkf.mpg.de “Towards efficient periodic coupled cluster theory calculations of solids and surfaces”

Thomas Jagau (Munich) thjapc@cup.uni-muenchen.de “Equation-of-motion coupled-cluster methods for shape and Feshbach resonances”

Mihály Kállay (Budapest) kallay@mail.bme.hu “Redundancy-free fragmentation-based local coupled-cluster approaches”

Eirik Kjørstad (NTNU) eirik.kjonstad@ntnu.no “Same-symmetry conical intersections with coupled cluster theory”

Henrik Koch (NTNU) henrik.koch@ntnu.no “Multi-level Hartree-Fock and coupled cluster theory”

Andreas Köhn (Stuttgart) koehn@theochem.uni-stuttgart.de “Quo vadis icMRCC?”

Anna Krylov (USC) anna.i.krylov@gmail.com “Non-adiabatic couplings in EOM-CC framework”

Simen Kvaal (Oslo) simen.kvaal@kjemi.uio.no “The bivariational principle: a rigorous Rayleigh–Ritz-like principle with applications to coupled-cluster theory”

Devin Matthews (Texas) dmatthews@utexas.edu “Simple spin-adaptation for equation-of-motion coupled-cluster theory”

Kaushik Nanda (USC) knanda@usc.edu “New theoretical tools for analyzing two-photon absorption cross-sections”

Frank Neese (MPI CEC) frank.neese@cec.mpg.de “Recent developments in local coupled cluster theory”

Marcel Nooijen (Waterloo) nooijen@uwaterloo.ca “Coupled cluster theory for periodic systems”

Thomas B. Pedersen (Oslo) t.b.pedersen@kjemi.uio.no “Local coupled-cluster theory with periodic boundary conditions”

Alexander Sokolov (CalTech) asokolov@caltech.edu “Towards robust multi-reference coupled cluster theory: can we learn anything from perturbation theory?”

John Stanton (Florida) jfstanton137@gmail.com “Some experiments with old ideas”

Stella Stopkowicz (Mainz) stella.stopkowicz@uni-mainz.de “Ground and excited states in strong magnetic fields with CC and EOM-CC theory”

David Tew (Bristol) David.Tew@bristol.ac.uk

Alex Thom (Cambridge) ajwt3@cam.ac.uk “Developments in stochastic coupled cluster theory”

Dominika Zgid (Michigan) dominika.zgid@gmail.com “Green's function embedding methods and their relationship to CC”