Title: “New Developments in Coupled-Cluster Theory”, July 19-23, 2021

Organizers:
Dr. Stella Stopkowicz, Department of Chemistry, University of Mainz, Germany
Prof. Thomas Jagau, Department of Chemistry, KU Leuven, Belgium
Prof. Anna Krylov, Department of Chemistry, University of Southern California, Los Angeles, USA

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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 many-body problem (Green functions, RPA, stochastic methods, etc);
- CC methods beyond electronic structure (nuclear problem, etc);
- extensions of CC theory driven by experiments (properties, spectroscopy modeling, etc)
- CC and machine learning

All talks are 30 min + 15 min discussion
Times are given as “Mountain Daylight Time / Central European Daylight Time”

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Program

Monday, July 19:

SESSION I (Chair: Stella Stopkowicz)
7:45 am / 3:45 pm Opening remarks
8:00 am / 4:00 pm Ali Alavi (MPI-FKF Stuttgart) *"Spin adaptation and the treatment of highly open-shell low-spin wavefunctions in FCIQMC"*
8:45 am / 4:45 pm Piotr Piecuch (Michigan State) *"Approaching exact quantum chemistry by semi-stochastic and selected-CI-driven coupled-cluster computations"*
9:30 am / 5:30 pm BREAK

SESSION II (Chair: Andreas Köhn)
10:00 am / 6:00 pm Jürgen Gauss (Mainz) *"Electron correlated calculation of energy and molecular properties: some recent developments"*
10:45 am / 6:45 pm Mihály Kallay (Budapest) *"Reducing the basis-set error of coupled-cluster methods by orbital-specific scaling"*
11:30 am / 7:30 pm BREAK
12:00 am / 8:00 pm Thomas Jagau (Leuven) "*Treatment of molecular Auger decay by means of complex-variable CC methods"*
12:45 pm / 8:45 pm END

Tuesday, July 20:

SESSION III (Chair: Devin Matthews)
8:00 am / 4:00 pm Simen Kvaal (Oslo) *"When there is no more room in Hilbert space: CC theory for bosons"*
8:45 am / 4:45 pm Fabijan Pavosevic (Yale) *"Multicomponent coupled cluster methods"*
9:30 am / 5:30 pm BREAK

SESSION IV (Chair: Anna Krylov)
10:00 am / 6:00 pm Daniel Crawford (Virginia Tech) *"Reduced-Scaling Coupled Cluster in the Frequency and Time Domains"*
10:45 am / 6:45 pm Thomas Bondo Pedersen (Oslo) *"Interpretation of coupled-cluster dynamics"*
11:30 am / 7:30 pm BREAK
12:00 am / 8:00 pm Eric Neuscamman (Berkeley) TBA
12:45 pm / 8:45 pm END

Wednesday, July 21:

SESSION V (Chair: Piotr Piecuch)
8:00 am / 4:00 pm Sonia Coriani (TU Denmark) *"Coupled cluster methods for spectroscopy: success stories and challenging cases"*
8:45 am / 4:45 pm Frank Neese (MPI-KOFO Mülheim) TBA
9:30 am / 5:30 pm BREAK

SESSION VI (Chair: Daniel Crawford)
10:00 am / 6:00 pm John Stanton (Florida) *"Normal v. EOM CC Methods for a Curious Problem: The Anomalous Anharmonicity of the CC Stretch in CCH"*
10:45 am / 6:45 pm Stella Stopkowicz (Mainz) *"New developments in finite-magnetic-field CC Theory"*
11:30 am / 7:30 pm BREAK
12:00 am / 8:00 pm Henrik Koch (SNS Pisa) *"Coupled cluster theory for molecular polaritons"*
12:45 pm / 8:45 pm END

Thursday, July 22:

SESSION VII (Chair: Henrik Koch)
8:00 am / 4:00 pm Francesco Evangelista (Emory) *"Electronic structure via unitary theories all the way down to the bottom"*
8:45 am / 4:45 pm Alexander Sokolov (Ohio State) *"Recent advances in algebraic diagrammatic construction theory"*
9:30 am / 5:30 pm BREAK

SESSION VIII (Chair: Sonia Coriani)
10:00 am / 6:00 pm Eirik Kjonstad (NTNU Trondheim) *"Non-adiabatic coupling elements: comparison of standard and similarity constrained coupled cluster methods"*
10:45 am / 6:45 pm Devin Matthews (Southern Methodist) "*Efficient Inclusion of Relaxation Effects in Core-Excitation Spectroscopy, and a Look at the Structure of 'Exact' Tensor Factorizations"*
11:30 am / 7:30 pm BREAK
12:00 am / 8:00 pm Lan Cheng (Johns Hopkins) *"Unitary Coupled-Cluster based excited-state methods"*
12:45 pm / 8:45 pm END

Friday, July 23:

SESSION IX (Chair: Jürgen Gauss)
8:00 am / 4:00 pm Karol Kowalski (PNNL) *"Downfolding of many-body Hamiltonians for strongly correlated molecular systems"*
8:45 am / 4:45 pm Marvin Lechner (MPI-KOFO Mülheim) *"Perturbative Approximations in MR-EOMCC Theory"*
9:30 am / 5:30 pm BREAK

SESSION X (Chair: Thomas Jagau)
10:00 am / 6:00 pm Andreas Köhn (Stuttgart) *"Perturbative approximations in internally-contracted multireference coupled-cluster theory"*
10:45 am / 6:45 pm Wim Klopper (Karlsruhe) *"Is the GW approximation a serious alternative to EOM-IP-CC theory?"*
11:30 am / 7:30 pm BREAK
12:00 am / 8:00 pm Anna Krylov (USC) *"Taming strong correlation by flipping one spin at a time"*
12:45 pm / 8:45 pm Closing remarks + discussion about future workshops
13:00 pm/ 9:00 pm END