

# Program: New Developments in Coupled-Cluster Theory 2019

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

Organizers:

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TSRC Hosts:

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## MONDAY

### Morning Session

08:00	08:15	Opening remarks		
08:15	09:00	Eric Neuscamman	Berkeley	Excited-State-Specific Electronic Structure Methods
09:00	09:45	Takeshi Sato	Tokyo	Time-dependent optimized coupled-cluster method for intense laser-driven multielectron dynamics
09:45	10:15	BREAK		
10:15	11:00	Simen Kvaal	Oslo	Two short talks on bivariational approaches for ab initio dynamics and the multireference problem
11:00	11:45	Thomas Bondo Pedersen	Oslo	Many-Electron Dynamics in Extreme Laser Pulses - A Challenge to Coupled-Cluster Theory

### Evening Session

19:00	19:45	Eugene DePrince	Florida	Time-dependent equation of motion coupled-cluster for linear spectroscopy
19:45	20:30	Andreas Grüneis	Vienna	TBA

## TUESDAY

### Afternoon Session

13:30	14:15	Thomas Jagau	Munich	TBA
14:15	15:00	Timothy Berkelbach	New York	Condensed-phase spectroscopy
15:00	15:30	BREAK		
15:30	16:15	Anna Krylov	USC	How to stay out of trouble in RIXS calculations within the equation-of-motion coupled-cluster damped response theory framework? Safe hitchhiking in the excitation manifold by means of core-valence separation.
16:15	16:40	Rasmus Faber	DTU Lyngby	Coupled Cluster Damped Response approaches for linear and non-linear X-ray spectroscopy
16:40	17:05	Pavel Pokhilko	USC	General framework for calculating spin-orbit couplings using spinless one-particle density matrices: Theory, application to EOM-CC, and analysis
18:30	19:15	TOWN TALK		

## WEDNESDAY

### Afternoon Session

13:30	14:15	Stella Stopkowicz	Mainz	Ground and excited states in strong magnetic fields with coupled cluster theory
14:15	15:00	Henrik Koch	NTNU	TBA
15:00	15:25	Eirik Kjønstad	NTNU	Nonadiabaticity in similarity constrained coupled cluster theory
15:25	15:55	BREAK		
15:55	16:40	John Stanton	Gainesville	Coupled-cluster theory, vibronic coupling and maybe a little bit about conical intersections
16:40	17:25	Robert Cave	Harvey Mudd college	Block Diagonalization Approaches for Transition Moments and Vibronic Coupling Matrix Elements

17:30 Group picture  
18:00 21:00 TSRC Picknick

#### THURSDAY

##### *Afternoon Session*

13:30	14:15	Frank Neese	Mülheim	On the ups and downs in the calculation of molecular (response) properties with domain based local pair natural orbital correlation methods
14:15	15:00	Róbert Izsák	Mühlheim	Domain-based Pair Natural Orbitals for Excited States Using the Similarity Transformed Equation of Motion Formalism
15:00	15:25	Franziska Engel	Mainz	Towards automatic code generation for PNO coupled-cluster methods with higher excitations
15:25	15:55	BREAK		
15:55	16:40	Mihály Kállay	Budapest	Optimization of the linear-scaling local natural orbital CCSD(T) method
16:40	17:25	Andreas Köhn	Stuttgart	Some aspects of making internally contracted multireference coupled-cluster theory more efficient

##### *Evening Session*

19:30	20:15	Peter Knowles	Cardiff	Coupled Cluster and Full CI for electrons, photons and vibrations
20:15	21:00	Jürgen Gauss	Mainz	Many-Body Expanded Full Configuration Interaction

#### FRIDAY

##### *Morning Session*

08:00	08:45	Florian Bischoff	Berlin	Coupled-Cluster in Real Space
08:45	09:30	Karol Kowalski	Pacific Northwest	Coupled-cluster formulations of the Green's function formalism: recent developments
09:30	10:00	BREAK		
10:00	10:25	Florian Hampe	Mainz	TBA
10:25	11:10	Wim Klopper	Karlsruhe	Ring coupled cluster theory and beyond
11:10	11:30	Closing		