

# Electronic Structure Methods for Time-Dependent, Frequency-Dependent and Spectroscopic Properties

Organizers: Joshua Kretchmer, Joonho Lee, and Daniel Nascimento  
March 24-26, 2026

## Tuesday AM

Georgia World Congress Center | Room B316

### Correlated Methods

J. Lee, D. Nascimento, Organizers | J. Kretchmer, Organizer, Presiding

**8:00 AM.** Introductory Remarks.

**8:05 AM.** Efficient multireference methods for excited states and spectroscopy.

**A. Sokolov**

**8:35 AM.** Dirac-Coulomb-Breit relativistic coupled-cluster methods for spectroscopic properties. **T. Zhang**, S.H. Yuwono, R.R. Li, S. Banerjee, E.F. Valeev, A. DePrince, X. Li

**8:50 AM.** Multireference equation-of-motion driven similarity renormalization group.

**Z. Zhao**, S. Li, F.A. Evangelista

**9:05 AM.** Recent progress in complex-energy electronic-structure methods. **T. Jagau**

**9:35 AM.** Development of relativistic equation-of-motion coupled-cluster methods. **Z. LIN**,

Y. Wu, X. Wang, S. Wang, S.H. Southworth, G. Doumy, L. Young, L. Cheng

**9:50 AM.** Intermission.

**10:15 AM.** Small tensor product distributed active space: Breaking the quadrillion determinant barrier in numerically exact configuration interaction. **X. Li**

**10:45 AM.** Regularized perturbation theory for ground state and excited state properties of ab initio solids. **M. Chen**, J. Lee

**11:00 AM.** Calculations of electronic excitations using variationally optimized orbitals and neural network accelerated selective ci. **H. Jonsson**

**11:15 AM.** Molecular response Properties from ab initio quantum electrodynamics.

**A. DePrince**, S.H. Yuwono

**11:45 AM.** Accelerating many-body green's function calculations for molecular systems via interacting-bath dynamical embedding theory. **C. Venturella**, J. Li, T. Zhu

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## Tuesday PM

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### **Nuclear Effects**

J. Lee, D. Nascimento, Organizers | J. Kretchmer, Organizer, Presiding

**2:00 PM.** Calculating the one- and two-dimensional electronic spectroscopy of different models of the hydrated electron. **B.J. Schwartz**, W. Borrelli

**2:30 PM.** Accurate solute-solvent models within hybrid QM/MM and QM methods in spectroscopy and dynamics. **G. Amante**, N. Rega

**2:45 PM.** Incorporating nuclear quantum effects into electronic excited-state simulations via constrained multicomponent TDDFT: Toward accurate excited-state dynamics and spectroscopic simulations. **Y. Wang**, Z. Chen, Y. Yang

**3:00 PM.** Real-time nuclear-electronic orbital quantum dynamics. **S. Hammes-Schiffer**

**3:30 PM.** Quantum molecular dynamics with electronic excitations employing exactly factorized wavefunctions. **J. Stetzler**, S. Garashchuk, V. Rassolov

**3:45 PM.** Intermission.

**4:15 PM.** From electronic structure to solvent effects: Ultrafast vibrational pathways in time-resolved spectroscopy. **N. Rega**

**4:45 PM.** Unambiguous spectral assignment via direct simulation of ultrafast observables. **A. Mehmood**, B. Levine

**5:00 PM.** Unveiling the origin of singlet-triplet coherence in bimetallic platinum complexes. **M. Taub**, D. Tang, L.X. Chen, X. Li

**5:15 PM.** Transient x-ray signatures of coupled structural and electronic motions during ultrafast excited-state intramolecular proton transfer. **N. Govind**, A. Nimmrich, A. Gomez, V. Freixas, C. Zhang, S. Mukamel, M.H. Khalil

**5:45 PM.** Scalable framework for NMR shielding computations: hybrid mpi/openmp and ri-accelerated finite-difference implementation at scf level and beyond. **X. Liu**, K. Nanda, M. Head-Gordon

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## Wednesday AM

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### Frequency-dependent and Excited State Techniques

J. Kretchmer, J. Lee, Organizers | D. Nascimento, Organizer, Presiding

**8:00 AM.** Time-dependent DFT for open-shell ground states. **J.M. Herbert**, A.K. Ojha

**8:30 AM.** Resolving equation-of-motion coupled-cluster band gaps of solids in the thermodynamic limit. **J. Li**, T. Zhu

**8:45 AM.** Ensemble time dependent density functional theory. **K.J. Daas**, S. Crisostomo, K. Burke

**9:00 AM.** Towards photochemistry with the resonating mean-field method. **S.M. Parker**

**9:30 AM.** Relativistic quantum electrodynamical time dependent density functional theory for spectroscopic properties in cavities and vacuum. **L. Konecny**

**9:45 AM.** Intermission.

**10:15 AM.** Approximate TDDFT methods for calculations on large systems. **C.M. Aikens**

**10:45 AM.** Resolving non-orthogonality in  $\Delta$ SCF and extending Excited-State theory from occupancy extrapolation. **Y. Shen**, Y. Fan, W. Yang

**11:00 AM.** Deconstructing chirality: Probing local and non-local effects in azobenzene derivatives with X-ray circular dichroism. **A. Khanna**, V.M. Freixas, L. Xu, J.R. Rouxel, N. Govind, M. Garavelli, S. Mukamel, S. Tretiak

**11:15 AM.** Electronic structure methods for electronic resonances. **K.B. Bravaya**

**11:45 AM.** Many-body perturbation theory in spectroscopy of solvated systems. **S. Kim**

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## Wednesday PM

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### Real-Time Dynamics

J. Lee, D. Nascimento, Organizers | J. Kretchmer, Organizer, Presiding

**2:00 PM.** Quantum electrodynamics time-dependent configuration interaction theory. J. Weidman, **B. Peyton**, Z. Stewart, A.K. Wilson

**2:30 PM.** Simulating magnetic field driven quantum dynamics using real-time London nuclear-electronic orbitals. **D. Tang**, A. Liu, T. Culpitt, S. Hammes-Schiffer, X. Li

**2:45 PM.** Modulating energy transfer in large two-dimensional plasmonic nanoarrays. **P.K. Verma**

**3:00 PM.** Correlated real-time electronic charge migration dynamics using the density matrix renormalization group. I. Wahyutama, M. Rano, **H.R. Larsson**

**3:30 PM.** Electron dynamics resulting from strong-field ionization of 1,3-cyclohexadiene via a few-cycle infrared pulse. **D.D. Jayasinghe**, K. Lopata

**3:45 PM.** Intermission.

**4:15 PM.** Relativistic real-time DFT: Probing light-induced ultrafast phenomena. **M. Repisky**, T. Moitra, L. Konecny, O. Neufeld, A. Rubio

**4:45 PM.** Development of spin-generalized real-time projected density matrix embedding theory. **M. Clothier**, S. Venkat, D. Yehorova, J. Kretchmer

**5:00 PM.** Large-scale real-time NEO-TDDFT simulations of ultrafast solvated electron dynamics. **A. Liu**, E. Lambros, R. Beck, T. Zhang, S. Hammes-Schiffer, X. Li

**5:15 PM.** First-principles open quantum dynamics for solids based on density-matrix formalism. **Y. Ping**

**5:45 PM.** Insight into photorelaxation processes through adiabatic/non-adiabatic AIMD simulations and wavelet transform analysis. **R. Carfora**, F. Coppola, P. Cimino, A. Petrone, N. Rega

# Electronic Structure Methods for Time-Dependent, Frequency-Dependent and Spectroscopic Properties

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## Thursday AM

Georgia World Congress Center | Room B310

### Real-time Methods for Spectroscopy

J. Kretchmer, J. Lee, Organizers | D. Nascimento, Organizer, Presiding

**8:00 AM.** Coupled cluster theory for chiroptical spectroscopy in the frequency and time domains. **T. Crawford**

**8:30 AM.** Electron dynamics with GPU accelerated real-time Tamm–Dancoff approximation (RT–TDA): Theory, algorithms and accuracy. **T. Knoll**

**8:45 AM.** Real-time time-dependent nonorthogonal configuration and orbital coupled propagation applied to modeling lanthanide oxide spectroscopy. **M. Moraes**, L.M. Thompson

**9:00 AM.** Spectroscopy and ultrafast dynamics of molecules in highly-excited states. **S. Bokarev**

**9:30 AM.** Time-dependent relativistic two-component equation-of-motion coupled-cluster for open-shell systems: TD-EA/IP-X2C-EOMCC. **P.S. Pathirage**, S.H. Yuwono, E. DePrince III

**9:45 AM.** Intermission.

**10:15 AM.** Time-dependent electronic structure tools for Coherent dynamics and nonlinear spectroscopy. **B.G. Levine**, A.S. Durden, B.S. Fales, T. Knoll, F. Liang, A. Mehmood, J. Suchan, Y. You

**10:45 AM.** Real-time time-dependent density functional theory simulations of core-hole induced valence electron dynamics. **T. Hua**, L. Kurkowski, K. Lopata

**11:00 AM.** Computing dynamical response of molecules in cavity using Time-Dependent approaches. **S.H. Yuwono**, K.A. Crouch, A. DePrince

**11:15 AM.** Modeling nonlinear optical spectroscopy signals in complex molecular systems. E. Lambertson, D. Bashirova, L. Allan, **T.J. Zuehlsdorff**

**11:45 AM.** Rovibrational states calculations of the H<sub>2</sub>O–HCN heterodimer with the multiconfiguration time dependent Hartree method. **H. Tajouo Tela**