Recent Progress in Theoretical Methods for Coupled Quantum Systems

Organizers: Kurt R. Brorsen, Yang Yang, Sharon Hammes-Shiffer

New Orleans, LA March 17-19, 2024

Sunday, March 17, 2024 | 8am – 12pm session

Ernest N. Morial Convention Center | R07

K. Brorsen, *Presiding*

8:00 AM. Coupled quantum systems via the exact factorization approach. **N. Maitra**

8:30 AM. Accurate pre-Born-Oppenheimer methods for solving the molecular Schroedinger equation. **R. Feldmann**, M. Reiher

9:00 AM. Toward accurate post-Born-Oppenheimer molecular simulations on quantum computers. **F. Pavosevic**

9:30 AM. A many-body perspective on proton polarization in solution. **E. Lambros**, S. Hammes-Schiffer, X. Li

9:45 AM. Efficient calculation of biexciton binding energies in semiconductor nanoparticles using stratified stochastic enumeration and multicomponent coupled cluster theory. C. Martin, **A. Chakraborty**

10:15 AM. Intermission.

10:30 AM. Ab initio theory of electrons coupled to lattice vibration. **J. Lee**

11:00 AM. Computing molecular vibrational spectra: Incorporating both quantum nuclear delocalization and mode coupling effects leads to significant improvement. **Y. Zhang**, Y. Wang, X. Xu, Z. Chen, Y. Yang

11:15 AM. Modeling polaritonics and plasmonics via real-time nuclear-electronic orbital approach. **T.E. Li**, S. Hammes-Schiffer

11:45 AM. On the nature of topological and geometric phases in coupled electron-nuclear dynamics around conical intersections. **L.M. Ibele**, F. Agostini

Sunday, March 17, 2024 | 2pm – 6pm session

Ernest N. Morial Convention Center | R07

Y. Yang, *Presiding*

2:00 PM. Exact factorization: A universal approach to non-adiabaticity. **E.K. Gross**

2:30 PM. Real-time nuclear-electronic orbital theory. **X. Li**, S. Hammes-Schiffer, A. Liu

3:00 PM. Modeling electron absorption spectra with nuclear quantum effects based on constrained nuclear-electronic orbital method. **X. Xu**

3:30 PM. Multicomponent second-order coupled cluster for accurate and efficient protonic excitations. **J. Fetherolf**

3:45 PM Intermission.

4:00 PM. Real-time neo-TDDFT for coupled quantum dynamics of electrons and protons in heterogeneous systems. **Y. Kanai**

4:30 PM. Theories and simulations of ultrafast processes in molecules. **F. Agostini**

5:00 PM. Efficient exact factorization-based trajectory methods: Restoring unique nuclear potentials and exploiting machine-learned electronic structure. **L.M. Dupuy**, N. Maitra

5:15 PM. Multicomponent Cholesky decomposition: Application to nuclear–electronic orbital theory. **A. Liu**, T. Zhang, S. Hammes-Schiffer, X. Li

5:30 PM. Calculation of vibrationally averaged properties with constrained multicomponent MP2. **G.B. Tucker**, D. Fowler, K. Brorsen

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Monday, March 18, 2024 | 8am – 12pm session
Ernest N. Morial Convention Center | R05
C. M. Isborn, *Presiding*

8:00 AM. Finite-temperature many-body perturbation theory for electrons and nuclei. **S. Hirata**

8:30 AM. Impact of electron-phonon interactions in 2D materials from first-principles theory and machine learning. **S. Sharifzadeh**

9:00 AM. Real-time molecular dipole switching dynamics in a cavity. **J. Weidman**, A.K. Wilson

9:15 AM. Non-adiabatic dynamics of plasmon-mediated photochemistry. **Y. Zhang**

9:30 AM. Nanometer-scale spatial and spectral mapping of exciton polaritons in structured plasmonic cavities. **D.J. Masiello**

9:45 AM. Nonadiabatic dynamics with electronic and vibrational strong couplings to light. **W. Dou**

10:00 AM. Intermission.

10:15 AM. Embedding theories for quantum simulations of materials on hybrid classical-quantum architectures. **G.A. Galli**

10:45 AM. Ab initio nonadiabatic molecular dynamics on many electronic states. **B.G. Levine**, A.S. Durden, M. Esch, F. Liang, W. Peng, Y. Shu

11:15 AM. Coherence maps and energy transfer dynamics from real-time path integral simulations. **N. Makri**

11:30 AM. Insight of hydrogen atom and proton transfer reactions through *ab initio* path integral molecular dynamics and real-time TDHF/TDDFT methods. **J. Zheng**

11:45 AM. Quantum wavepacket dynamics on ion-trap quantum computers: New algorithms to compute vibrational properties of anharmonic hydrogen bonds. **S.S. Iyengar**, D. Saha, M. Revelle, P. Richerme, A. Sabry

Monday, March 18, 2024 | 2pm – 6pm session
Ernest N. Morial Convention Center | R05
S. Sharifzadeh, *Presiding*

2:00 PM. Decoding signatures of large amplitude vibrational motions: Exploring the stories encoded in vibrational spectra. **A.B. McCoy**, P. Moonkaen, Y.M. Hassan, G. Jacobson

2:30 PM. Coupling between vibronic, environmental, and electronic degrees of freedom in simulations of optical spectroscopy. **C. Isborn**

3:00 PM. Local diabatic representation of conical intersection dynamics. **B. Gu**

3:15 PM. Topological classification of chemical reactions: A new tool to understand chemical reactivity. **L. Muechler**

3:30 PM. Photophysics of solvated molecules: Coupling electronic with nuclear and solvent degrees of freedom. **P. de Silva**

3:45 PM. Intermission.

4:00 PM. On the creation of a hierarchy of methods for nonadiabatic molecular dynamics. **B.F. Curchod**

4:30 PM. Quantum optimal control for differentiating vibrational spectra of isotopologues. **L. McCaslin**

4:45 PM. Integrating quantum decoherence within Ehrenfest: A paradigm for multistate dynamics. **F. Liang**, B.G. Levine

5:00 PM. Delocalization-induced tuning of electron-phonon and electron-vibration interactions in chlorophyll proteins. G. Grechishnikova, L.V. Slipchenko, L. Huang, **M. Reppert**

5:15 PM. Hop to it: cumulative probabilities make surface hopping simulations cheaper and more reproducible. **S.M. Parker**

5:30 PM. Stochastic CC2 method to electron excitation for very large systems. **C. Zhao**, W. Dou, J. Lee

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Tuesday, March 19, 2024 | 8am – 12pm session

Ernest N. Morial Convention Center | R05

F. Pavosevic, *Presiding*

8:00 AM. Nonlinearities and high-harmonic generation with strongly coupled light-matter systems. **P. Narang**

8:30 AM. Resonance theory and quantum dynamics simulations of vibrational polariton chemistry. **P. Huo**

9:00 AM. Excitonic polariton and dark states for many molecules in the Fabry-Perot cavity. **Y. Shao**, Z. Pei, C. Lander, Y. Zhang, P. Huo

9:30 AM. Quantum-electrodynamic electron transfer reaction: A perspective beyond cavity quantum electrodynamics. **L. Hsu**, Y. Wei

10:00 AM. Intermission.

10:15 AM. Molecular polaritons as quantum impurity problems. **J. Yuen Zhou**

10:45 AM. Ab initio cavity quantum electrodynamics. **A. DePrince**

11:15 AM. First-principle approaches to strong light-matter coupling in molecular systems. **J. Flick**

Tuesday, March 19, 2024 | 2pm – 6pm session

Ernest N. Morial Convention Center | R09

Joint Session with Current Trends in Polariton Chemistry

R.F. Ribeiro, *Presiding*

2:00 PM. Toward simulations of quantum dynamics at complex plasmonic interfaces. **M. Sukharev**

2:30 PM. Linear and nonlinear response of cavity polaritons: Exciton scattering approach. **V.Y. Chernyak**

3:00 PM. Ab initio methods for polariton chemistry. **J.J. Foley**

3:30 PM. Polaritonic chemistry and the impact of dephasing effects in molecular ensembles. **M. Kowalewski**, E. Davidsson, L. Borges

3:50 PM. Intermission.

4:10 PM. Quantum modeling of propagating plexcitons in two-dimensional materials. **M. Mosquera**

4:40 PM. Polaritonic chemistry from micrometer to nanometer scales. **J. Feist**

5:10 PM. Cavity control of molecular spectroscopy and photophysics. **S. Mukamel**, Y. Gu, B. Gu, V.Y. Chernyak

5:40 PM. Quantum coherence in cavity polariton chemistry. **J. Cao**