

In Honor of Gregory Voth's 65th Birthday: From Quantum Dynamics to Ultra Coarse-Graining, and Everything in Between

Organizers: R. Kumar, J. Li, F. Paesani, and D. R. Reichman

New Orleans, LA

March 17-21, 2024

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

Ernest N. Morial Convention Center | R06

F. Paesani, *Presiding*

8:00 AM. Introductory Remarks.

8:05 AM. Classical molecular dynamics simulations of electronically non-adiabatic processes. **W.H. Miller**

8:35 AM. Science Inspired by Greg Voth. **D.R. Reichman**

8:55 AM. Real-time path integral methods and state-to-state pathways of quantum dynamics. **N. Makri**

9:15 AM. Intermission.

9:35 AM. Fermi's Golden Rule based rates for exciton and electron transfer and nonradiative decay processes due to derivative coupling. **S.J. Jang**

9:55 AM. Novel path-space framework for mixed quantization: from quantum dynamics to classical dynamics and everything in between. **N. Ananth**

10:15 AM. Atom-centered density matrix propagation (ADMP) with post-Hartree-Fock accuracy: Computational improvements through an adaptive and general transfer machine learning protocol with reduced training needs. **S.S. Iyengar**

10:35 AM. Intermission.

10:55 AM. Recent advances in methods for photodynamics simulations — NACs for free. **D.G. Truhlar**, Y. Shu, L. Zhang, X. Zhao, X. Xu

11:15 AM. Electron transfer, angular momentum, and the CISS effect. **J.E. Subotnik**

11:35 AM. New phase space formulation of quantum mechanics for nonadiabatic dynamics. **J. Liu**

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

Ernest N. Morial Convention Center | R06

Quantum Dynamics | D. R. Reichman, *Presiding*

2:00 PM. My long history with Greg Voth. **J.P. Simons**

2:30 PM. Exciton-polariton dynamics in colloidal quantum dots nanocrystals. **E. Rabani**

2:50 PM. Quantum diffusion in organic materials: Disorder, phonons, and photons. **J. Cao**

3:10 PM. How biology has evolved to manipulate vibronic coupling to steer energy transfer in photosynthesis. **G.S. Engel**

3:30 PM. Intermission.

3:50 PM. Real-time nuclear-electronic orbital quantum dynamics. **S. Hammes-Schiffer**

4:10 PM. Influence of structural disorder on the spatial heterogeneity of singlet fission rates in rubrene crystals. S.T. Roberts, **P.J. Rossky**, M.T. Zanni

4:30 PM. Ab initio surface chemistry with chemical accuracy. **T.C. Berkelbach**

4:50 PM. Intermission.

5:10 PM. Skewed paraboloids of molecular electrostatics and charge transfer: From polarizable spheres to proteins. **D.V. Matyushov**

5:30 PM. Simulating quantum critical molecular assemblies: From path integrals to matrix product states. **P. Roy**, T. Serwatka

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Monday, March 18, 2024 | 8am – 12pm session

Ernest N. Morial Convention Center | R06
Molecular Interactions and Dynamics | J. Li, *Presiding*

- 8:00 AM.** Inorganic aqueous interfaces from first principles simulations. **G.A. Galli**
- 8:30 AM.** Exploring graphene oxide-solvent interfaces. **R. Kumar**, G. Azom, R. David
- 8:50 AM.** Modelling the uptake, transport and separation of multiply charged ions through MoS₂ membranes. **G.C. Schatz**
- 9:10 AM.** Intermission.
- 9:50 AM.** Accurate modeling of many-body energies in water clusters and applications to liquid water and ice. **S. Xantheas**, K.M. Herman, A. Stone
- 10:10 AM.** Raising the bar for molecular simulations with data-driven many-body potentials. **F. Paesani**
- 10:30 AM.** Intermission.
- 10:50 AM.** Exploring spectral signatures of proton migration in protonated water clusters. **A.B. McCoy**, J. Finney, P. Moonkaen
- 11:10 AM.** Highly concentrated acid solutions: From proton hopping to the bulk viscosity. **M.D. Fayer**, I. Kacenauskaite, M.M. Cohen
- 11:30 AM.** Theory and applications of shapeGMM, a probabilistic structural clustering method for macromolecular simulation. **M. McCullagh**

Monday, March 18, 2024 | 2pm – 6pm session

Ernest N. Morial Convention Center | R06
Biomolecular Systems | R. Kumar, *Presiding*

- 2:00 PM.** Microtubules' bends, cryo-cool ribosomes, and wet proteins. **K. Grubmueller**, M. Igaev, B. Lars V., L. Heinz
- 2:30 PM.** The lipid-dependent thermodynamics of GPCR signaling. **E. Lyman**
- 2:50 PM.** Mechanism of membrane curvature induced by SNX1: Insights from molecular dynamics simulations. Z. Liao, **J. Fan**
- 3:10 PM.** PIP₂ clustering with CHARMM36 and Martini3. **R. Pastor**, Z. Jarin, R.M. Venable, K. Han
- 3:30 PM.** Intermission.
- 3:50 PM.** Trapping an amyloid oligomer by working against nature. **M.T. Zanni**
- 4:10 PM.** Self-assembly of the tau protein: Liquid-liquid phase separation and fibrillization. **J.E. Shea**
- 4:30 PM.** Reshaping cells across the tree of life. **A. Saric**
- 4:50 PM.** Intermission.
- 5:10 PM.** Importance of electrostatics for chemical transformations: Enzymes, nanocages, and microdroplet chemistry. **T.L. Head-Gordon**
- 5:30 PM.** P-type ion pump: Simulations and theory. **B. Roux**

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

Ernest N. Morial Convention Center | R06

Free-energy Landscapes and Coarse Graining | G. M. Hocky, *Presiding*

8:20 AM. Reliable free energies from first principles with adaptive force matching. **F. Wang**

8:40 AM. Impact of unstirred water layer on the permeation of small molecule drugs. C. Kang, M. Bernaldez, **R. Sun**

9:00 AM. Exploring the temporal evolution of the HIV viral population under drug selection pressure. **R.M. Levy**

9:20 AM. Intermission.

9:40 AM. Computational microscope that can zoom: Multiscale modeling for biomolecular complexes. **J. Li**

10:00 AM. Maximum entropy theory of multiscale coarse-graining via matching thermodynamic forces: Application to a molecular crystal. **S. Izvekov**, M. Kroonblawd, J.P. Larentzos, J. Brennan, B.M. Rice

10:20 AM. Progress towards predictive coarse-grained models. **W.N. Noid**

10:40 AM. Transferable coarse-grained models using relative entropy optimization. **M. Shell**

11:00 AM. Intermission.

11:20 AM. Bottom-up coarse-grained models of biological macromolecules: A new method to access conformational transitions from molecular dynamics simulations. **T. Bidone**

11:40 AM. Understanding dynamics in coarse-grained models using excess entropy scaling. **J. Jin**, G.A. Voth

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

Ernest N. Morial Convention Center | R06

Free-energy Landscapes and Coarse Graining | R. Sun, *Presiding*

2:00 PM. Using coarse-graining to design autonomous computing materials. **R. Hernandez**, X. Wei, Y. Zhao, E. Harazinska

2:20 PM. Backmapping method to convert a coarse-grained system into a fully atomistic one. **S. Kim**

2:40 PM. Understanding the photochemical reactions in biomolecules through multiscale simulations. **R. Liang**

3:00 PM. Intermission.

3:20 PM. Discovering optimal kinetic pathways for macromolecular assembly. **M.E. Johnson**

3:40 PM. Integrating molecular dynamics simulations and deep learning models to investigate morphological transitions in biomacromolecular complexes. **A.J. Pak**

4:00 PM. From chemical identity to Boltzmann ensembles for proteins, RNA and crystals with generative AI and statistical mechanics. **P. Tiwary**

4:20 PM. Intermission.

4:40 PM. Sloppy yet precise control of non-equilibrium materials. **S. Vaikuntanathan**

5:00 PM. Recent advances in the theory and simulation of rare events. **D. Limmer**

5:20 PM. Good rates from bad coordinates. N. Mazzaferro, P. Cossio, **G.M. Hocky**

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Wednesday, March 20, 2024 | 8am – 12pm session

Ernest N. Morial Convention Center | R06

Everything in Between | J. Li, *Presiding*

8:00 AM. Non-equilibrium electron dynamics from real-time quantum embedding. **J. Kretchmer**

8:20 AM. Quantum diffusion of atoms trapped in solid parahydrogen. **I. Muddasser**, A. Nguyen, D.T. Anderson

8:40 AM. Molecular dynamics studies of the kinetics and mechanism of solid-phase epitaxy in oxides.
J.R. Schmidt

9:00 AM. Intermission.

9:20 AM. Accurate and efficient order- N framework for hybrid DFT based *ab initio* molecular dynamics of heterogeneous finite-gap condensed-phase systems. H. Ko, Z.M. Sparrow, J. Zhang, **R.A. Distasio**

9:40 AM. Non-empirical tight binding theory. **A.V. Mironenko**

10:00 AM. Light induced spin-exciton interaction. **T. Xu**

10:20 AM. Intermission.

10:40 AM. Low and high frequency vibrations synergistically enhance singlet exciton fission through robust vibronic resonances. **A. Bhattacharyya**, A. Sahu, S. Patra, V. Tiwari

11:00 AM. Multiscale simulations of HIV-1 fusion peptide insertion into T-cell membrane mimic.
S. Gnanakaran

11:20 AM. Statistical estimates of biophysical descriptors of nanoparticle protein coronas. V.K. Annapoorani, O. Petrisor, **N. Buchete**