Stanford



Thomas E. Markland

Professor of Chemistry

CONTACT INFORMATION

- **Administrative Contact**

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Bio

BIO

Professor Tom Markland focuses on problems at the interface of quantum mechanics and statistical mechanics, with applications ranging from chemistry and biology to geology and materials science. Markland Group research frequently explores theories of hydrogen bonding, the interplay between structure and dynamics, systems with multiple time and length-scales, and quantum mechanical effects. Particular current interests include proton and electron transfer in materials and enzymatic systems, atmospheric isotope separation, and the control of catalytic chemical reactivity in heterogeneous environments.

Thomas E. Markland studied chemistry at Balliol College, University of Oxford (MChem 2006), where as a Brackenbury Scholar he performed thesis work in the area of non-adiabatic dynamics. He continued at Oxford (D.Phil. 2009), working in quantum dynamics under the supervision of Professor David Manolopoulos. Together, the two developed an approach to allow quantum effects of nuclei to be included in condensed phase simulation at near classical computational cost, as well as elucidating isotope effects observed in liquids. Next, during postdoctoral work with Bruce Berne at Columbia University, Professor Markland focused on structure and dynamics in classical and quantum biophysical systems. He moved to Stanford in 2011 as an Assistant Professor in the Department of Chemistry and was promoted to Associate Professor with tenure in 2018. He has received recognition in a number of awards, including a Research Corporation Cottrell Scholarship, Alfred P. Sloan Research Fellowship, Terman Fellowship, Hellman Faculty Scholarship, the ACS OpenEye Outstanding Junior Faculty Award, the NSF CAREER award, the Camille Dreyfus Teacher-Scholar award, the H&S Dean's Award for Distinguished Teaching, the Kavli Emerging Leader in Chemistry Lectureship, and the ACS Early Career Award in Theoretical Chemistry.

Research in the Markland Group lies in the application and development of theoretical methods to model condensed phase systems, with a particular emphasis on the role of quantum mechanical effects. Treatment of these problems requires a range of theoretical approaches as well as molecular mechanics and ab initio simulations. The group is particularly interested in developing and applying methods based on the path integral formulation of quantum mechanics to include quantum fluctuations such as zero-point energy and tunneling in the dynamics of reactive condensed phase systems.

The group has also developed methods to treat non-equilibrium excited state dynamics by exploiting the combination of quantum-classical theory and quantum master equation approaches.

Work in the Markland Group has already provided insights into several systems, including reactions in liquids and enzymes, and the quantum liquid–glass transition. Group members have also introduced methods to perform path integral calculations at near classical computational cost, expanding the ability to treat large-scale condensed phase systems.

ACADEMIC APPOINTMENTS

- Professor, Chemistry
- Member, Bio-X
- Principal Investigator, Stanford PULSE Institute

ADMINISTRATIVE APPOINTMENTS

- Member, Stanford PULSE Institute, SLAC National Accelerator Laboratory, (2014- present)

HONORS AND AWARDS

- Christ’s College Distinguished Visiting Scholar, Christ's College, Cambridge (2026)
- ACS Early Career Award in Theoretical Chemistry, American Chemical Society (2021)
- Kavli Emerging Leader in Chemistry Lectureship, Kavli Foundation (2019)
- Camille Dreyfus Teacher-Scholar Award, Camille and Henry Dreyfus Foundation (2017)
- Terman Fellow, Stanford University (2017)
- NSF CAREER award, National Science Foundation (2016)
- Cottrell Scholar, Research Corporation for Science Advancement (2015)
- Dean's Award for Distinguished Teaching, Stanford University School of Humanities & Sciences (2015)
- Hellman Faculty Scholar, Stanford University (2014)
- OpenEye Outstanding Junior Faculty Award, American Chemical Society (2014)
- Sloan Research Fellowship, Alfred P. Sloan Foundation (2014)
- Terman Fellow, Stanford University (2012)
- Coulson Prize, Royal Society of Chemistry (2009)

PROFESSIONAL EDUCATION

- Postdoc, Columbia University , Theoretical Chemistry (2010)
- DPhil, University of Oxford , Chemistry (2009)
- MChem, University of Oxford , Chemistry (2006)

LINKS

- The Markland Group: https://www.marklandlab.com

Research & Scholarship

CURRENT RESEARCH AND SCHOLARLY INTERESTS

Our research centers on problems at the interface of quantum and statistical mechanics. Particular themes that occur frequently in our research are hydrogen bonding, the interplay between structure and dynamics, systems with multiple time and length-scales and quantum mechanical effects. The applications of our methods are diverse, ranging from chemistry to biology to geology and materials science. Particular current interests include proton

and electron transfer in fuel cells and enzymatic systems, atmospheric isotope separation and the control of catalytic chemical reactivity using electric fields.

Treatment of these problems requires a range of analytic techniques as well as molecular mechanics and ab initio simulations. We are particularly interested in developing and applying methods based on the path integral formulation of quantum mechanics to include quantum fluctuations such as zero-point energy and tunneling in the dynamics of liquids and glasses. This formalism, in which a quantum mechanical particle is mapped onto a classical "ring polymer," provides an accurate and physically insightful way to calculate reaction rates, diffusion coefficients and spectra in systems containing light atoms. Our work has already provided intriguing insights in systems ranging from diffusion controlled reactions in liquids to the quantum liquid-glass transition as well as introducing methods to perform path integral calculations at near classical computational cost, expanding our ability to treat large-scale condensed phase systems.

Teaching

COURSES

2026-27

- Computational Electronic Structure of Molecular Systems: CHEM 161, CHEM 261 (Win)
- Department Colloquium: CHEM 300 (Win)
- Linking the Molecular to the Macroscopic: Foundations of Physical Chemistry: CHEM 171 (Spr)
- Physical Chemistry Seminar: CHEM 379 (Win)

2025-26

- Department Colloquium: CHEM 300 (Win)
- Linking the Molecular to the Macroscopic: Foundations of Physical Chemistry: CHEM 171 (Spr)
- Physical Chemistry Seminar: CHEM 379 (Win)

2024-25

- Computational Chemistry: CHEM 161, CHEM 261 (Win)
- Department Colloquium: CHEM 300 (Aut, Win, Spr)
- Foundations of Physical Chemistry: CHEM 171 (Spr)
- Physical Chemistry Seminar: CHEM 379 (Aut, Win, Spr)

2023-24

- Computational Chemistry: CHEM 161, CHEM 261 (Win)
- Department Colloquium: CHEM 300 (Aut, Win, Spr)
- Foundations of Physical Chemistry: CHEM 171 (Spr)
- Physical Chemistry Seminar: CHEM 379 (Aut, Win, Spr)

STANFORD ADVISEES

Doctoral Dissertation Reader (AC)

Jan Estrada Pabon, Steven Fried, Nicholas Juntunen, John Walters, Nancy Zhu

Postdoctoral Faculty Sponsor

Anna Bui

Doctoral Dissertation Advisor (AC)

Frank Hu

Publications

PUBLICATIONS

- **Streamlining analysis and design of two-dimensional electronic spectroscopy using machine learning.** *The Journal of chemical physics*
  Hausman, N. I., Kelly, J., Chen, M. S., Hu, F., Lee, A., Montoya-Castillo, A., Schlau-Cohen, G. S., Markland, T. E.
  2026; 165 (7)

- **Pushing the Limits of One-Dimensional NMR Spectroscopy for Automated Structure Elucidation Using Artificial Intelligence.** *Journal of chemical information and modeling*
  Hu, F., Tubb, J. M., Argyropoulos, D., Golotvin, S., Elyashberg, M., Rotskoff, G. M., Kanan, M. W., Markland, T. E.
  2026

- **Accuracy and Efficiency Benchmarks of Pretrained Machine Learning Potentials for Molecular Simulations.** *Journal of chemical theory and computation*
  Eastman, P., Pretti, E., Markland, T. E.
  2026

- **Efficient simulation of optical spectra via machine learning and physical decomposition of environmental effects.** *The Journal of chemical physics*
  Snider, A., Chen, M. S., Markland, T. E., Isborn, C. M.
  2026; 164 (13)

- **Label-Free Optical Differentiation of Single Diffusing Amino Acids at Picomolar Concentrations.** *Research square*
  Goldsmith, R., Rasch, J., Clayborn, A., Sole-Barber, D., Wan, S., Saavedra, C., Fairhall, A., Hu, F., Bartz, J., Podorova, Y., Bergsten, A., Young, Z. D., Barrera, et al
  2026

- **Ion-exchange-mediated pre-association gates interfacial PCET** *CHEM*
  Lewis, N. B., Kelly, J., Gardner, J. G., Razdan, N. K., Ardo, S., Markland, T. E., Surendranath, Y.
  2026; 12 (3)

- **Two-dimensional electronic spectra from trajectory-based dynamics: Pure-state Ehrenfest, spin-mapping, and mean classical path approaches.** *The Journal of chemical physics*
  Lieberherr, A. Z., Kelly, J., Runeson, J. E., Markland, T. E., Manolopoulos, D. E.
  2025; 163 (21)

- **Proton-Transfer Kinetics at Liquid-Liquid Interfaces.** *Journal of the American Chemical Society*
  D'Antona, N., Kelly, J., Barnard, N., Ardo, S., Wang, Y., Surendranath, Y., Markland, T. E., Kempler, P. A., Boettcher, S. W.
  2025

- **Two-Dimensional Electronic Spectroscopy in the Condensed Phase Using Equivariant Transformer Accelerated Molecular Dynamics Simulations.** *The journal of physical chemistry letters*
  Kelly, J., Hu, F., Damiani, A., Chen, M. S., Snider, A., Son, M., Lee, A., Gupta, P., Montoya-Castillo, A., Zuehlsdorff, T. J., Schlau-Cohen, G. S., Isborn, C. M., Markland, et al
  2025: 5561-5569

- **Beyond the Vibrational Stark Effect: Unraveling the Large Redshifts of Alkyne C-H Bond in Solvation Environments.** *Journal of the American Chemical Society*
  Zheng, C., Mao, Y., Markland, T. E., Boxer, S. G.
  2025

- **Accurate and Efficient Structure Elucidation from Routine One-Dimensional NMR Spectra Using Multitask Machine Learning.** *ACS central science*
  Hu, F., Chen, M. S., Rotskoff, G. M., Kanan, M. W., Markland, T. E.
  2024; 10 (11): 2162-2170

- **Nutmeg and SPICE: Models and Data for Biomolecular Machine Learning.** *Journal of chemical theory and computation*
  Eastman, P., Pritchard, B. P., Chodera, J. D., Markland, T. E.

2024

- **TorchMD-Net 2.0: Fast Neural Network Potentials for Molecular Simulations.** *Journal of chemical theory and computation*
  Pelaez, R. P., Simeon, G., Galvelis, R., Mirarchi, A., Eastman, P., Doerr, S., Tholke, P., Markland, T. E., De Fabritiis, G.
  2024
- **TorchMD-Net 2.0: Fast Neural Network Potentials for Molecular Simulations.** *ArXiv*
  Pelaez, R. P., Simeon, G., Galvelis, R., Mirarchi, A., Eastman, P., Doerr, S., Thölke, P., Markland, T. E., De Fabritiis, G.
  2024
- **Enhancing Protein-Ligand Binding Affinity Predictions Using Neural Network Potentials.** *Journal of chemical information and modeling*
  Sabanés Zariquiey, F., Galvelis, R., Gallicchio, E., Chodera, J. D., Markland, T. E., De Fabritiis, G.
  2024
- **OpenMM 8: Molecular Dynamics Simulation with Machine Learning Potentials.** *The journal of physical chemistry. B*
  Eastman, P., Galvelis, R., Peláez, R. P., Abreu, C. R., Farr, S. E., Gallicchio, E., Gorenko, A., Henry, M. M., Hu, F., Huang, J., Krämer, A., Michel, J., Mitchell, et al
  2023
- **NNP/MM: Accelerating Molecular Dynamics Simulations with Machine Learning Potentials and Molecular Mechanics.** *Journal of chemical information and modeling*
  Galvelis, R., Varela-Rial, A., Doerr, S., Fino, R., Eastman, P., Markland, T. E., Chodera, J. D., De Fabritiis, G.
  2023
- **Developing machine-learned potentials to simultaneously capture the dynamics of excess protons and hydroxide ions in classical and path integral simulations.** *The Journal of chemical physics*
  Atsango, A. O., Morawietz, T., Marsalek, O., Markland, T. E.
  2023; 159 (7)
- **Elucidating the Role of Hydrogen Bonding in the Optical Spectroscopy of the Solvated Green Fluorescent Protein Chromophore: Using Machine Learning to Establish the Importance of High-Level Electronic Structure.** *The journal of physical chemistry letters*
  Chen, M. S., Mao, Y., Snider, A., Gupta, P., Montoya-Castillo, A., Zuehlsdorff, T. J., Isborn, C. M., Markland, T. E.
  2023: 6610-6619
- **Electron transfer at electrode interfaces via a straightforward quasiclassical fermionic mapping approach.** *The Journal of chemical physics*
  Jung, K. A., Kelly, J., Markland, T. E.
  2023; 159 (1)
- **Building insightful, memory-enriched models to capture long-time biochemical processes from short-time simulations.** *Proceedings of the National Academy of Sciences of the United States of America*
  Dominic, A. J., Sayer, T., Cao, S., Markland, T. E., Huang, X., Montoya-Castillo, A.
  2023; 120 (12): e2221048120
- **A derivation of the conditions under which bosonic operators exactly capture fermionic structure and dynamics.** *The Journal of chemical physics*
  Montoya-Castillo, A., Markland, T. E.
  2023; 158 (9): 094112
- **An accurate and efficient Ehrenfest dynamics approach for calculating linear and nonlinear electronic spectra.** *The Journal of chemical physics*
  Atsango, A. O., Montoya-Castillo, A., Markland, T. E.
  2023; 158 (7): 074107
- **Data-Efficient Machine Learning Potentials from Transfer Learning of Periodic Correlated Electronic Structure Methods: Liquid Water at AFQMC, CCSD, and CCSD(T) Accuracy.** *Journal of chemical theory and computation*
  Chen, M. S., Lee, J., Ye, H. Z., Berkelbach, T. C., Reichman, D. R., Markland, T. E.
  2023
- **SPICE, A Dataset of Drug-like Molecules and Peptides for Training Machine Learning Potentials.** *Scientific data*
  Eastman, P., Behara, P. K., Dotson, D. L., Galvelis, R., Herr, J. E., Horton, J. T., Mao, Y., Chodera, J. D., Pritchard, B. P., Wang, Y., De Fabritiis, G., Markland, T. E.

2023; 10 (1): 11

- **2D spectroscopies from condensed phase dynamics: Accessing third-order response properties from equilibrium multi-time correlation functions.** *The Journal of chemical physics*
  Jung, K. A., Markland, T. E.
  2022; 157 (9): 094111

- **Optically Induced Anisotropy in Time-Resolved Scattering: Imaging Molecular-Scale Structure and Dynamics in Disordered Media with Experiment and Theory.** *Physical review letters*
  Montoya-Castillo, A., Chen, M. S., Raj, S. L., Jung, K. A., Kjaer, K. S., Morawietz, T., Gaffney, K. J., van Driel, T. B., Markland, T. E.
  2022; 129 (5): 056001

- **Solvent Organization and Electrostatics Tuned by Solute Electronic Structure: Amide versus Non-Amide Carbonyls.** *The journal of physical chemistry. B*
  Fried, S. D., Zheng, C., Mao, Y., Markland, T. E., Boxer, S. G.
  2022

- **A two-directional vibrational probe reveals different electric field orientations in solution and an enzyme active site.** *Nature chemistry*
  Zheng, C., Mao, Y., Kozuch, J., Atsango, A. O., Ji, Z., Markland, T. E., Boxer, S. G.
  2022

- **A framework for automated structure elucidation from routine NMR spectra.** *Chemical science*
  Huang, Z., Chen, M. S., Woroch, C. P., Markland, T. E., Kanan, M. W.
  2021; 12 (46): 15329-15338

- **A framework for automated structure elucidation from routine NMR spectra** *CHEMICAL SCIENCE*
  Huang, Z., Chen, M. S., Woroch, C. P., Markland, T. E., Kanan, M. W.
  2021

- **Characterizing and Contrasting Structural Proton Transport Mechanisms in Azole Hydrogen Bond Networks Using Ab Initio Molecular Dynamics.** *The journal of physical chemistry letters*
  Atsango, A. O., Tuckerman, M. E., Markland, T. E.
  2021: 8749-8756

- **AENET-LAMMPS and AENET-TINKER: Interfaces for accurate and efficient molecular dynamics simulations with machine learning potentials** *JOURNAL OF CHEMICAL PHYSICS*
  Chen, M. S., Morawietz, T., Mori, H., Markland, T. E., Artrith, N.
  2021; 155 (7): 074801

- **Persistent Homology Metrics Reveal Quantum Fluctuations and Reactive Atoms in Path Integral Dynamics.** *Frontiers in chemistry*
  Hu, Y., Ounkham, P., Marsalek, O., Markland, T. E., Krishmoorthy, B., Clark, A. E.
  2021; 9: 624937

- **Exploiting Machine Learning to Efficiently Predict Multidimensional Optical Spectra in Complex Environments.** *The journal of physical chemistry letters*
  Chen, M. S., Zuehlsdorff, T. J., Morawietz, T., Isborn, C. M., Markland, T. E.
  2020: 7559–68

- **On the advantages of exploiting memory in Markov state models for biomolecular dynamics.** *The Journal of chemical physics*
  Cao, S., Montoya-Castillo, A., Wang, W., Markland, T. E., Huang, X.
  2020; 153 (1): 014105

- **Quantum kinetic energy and isotope fractionation in aqueous ionic solutions.** *Physical chemistry chemical physics : PCCP*
  Wang, L. n., Ceriotti, M. n., Markland, T. E.
  2020

- **Elucidating the Proton Transport Pathways in Liquid Imidazole with First-Principles Molecular Dynamics.** *The journal of physical chemistry letters*
  Long, Z. n., Atsango, A. O., Napoli, J. A., Markland, T. E., Tuckerman, M. E.
  2020: 6156–63

- **Excited state diabatization on the cheap using DFT: Photoinduced electron and hole transfer.** *The Journal of chemical physics*
  Mao, Y. n., Montoya-Castillo, A. n., Markland, T. E.
  2020; 153 (24): 244111
- **Resolving Heterogeneous Dynamics of Excess Protons in Aqueous Solution with Rate Theory.** *The journal of physical chemistry. B*
  Roy, S. n., Schenter, G. K., Napoli, J. A., Baer, M. D., Markland, T. E., Mundy, C. J.
  2020
- **Accurate and efficient DFT-based diabatization for hole and electron transfer using absolutely localized molecular orbitals.** *The Journal of chemical physics*
  Mao, Y., Montoya-Castillo, A., Markland, T. E.
  2019; 151 (16): 164114
- **Tracking Aqueous Proton Transfer by Two-Dimensional Infrared Spectroscopy and ab Initio Molecular Dynamics Simulations** *ACS CENTRAL SCIENCE*
  Yuan, R., Napoli, J. A., Yan, C., Marsalek, O., Markland, T. E., Fayer, M. D.
  2019; 5 (7): 1269–77
- **Tracking Aqueous Proton Transfer by Two-Dimensional Infrared Spectroscopy and ab Initio Molecular Dynamics Simulations.** *ACS central science*
  Yuan, R., Napoli, J. A., Yan, C., Marsalek, O., Markland, T. E., Fayer, M. D.
  2019; 5 (7): 1269-1277
- **i-PI 2.0: A universal force engine for advanced molecular simulations** *COMPUTER PHYSICS COMMUNICATIONS*
  Kapil, V., Rossi, M., Marsalek, O., Petraglia, R., Litman, Y., Spura, T., Cheng, B., Cuzzocrea, A., Meissner, R. H., Wilkins, D. M., Helfrecht, B. A., Juda, P., Bienvenue, et al
  2019; 236: 214–23
- **Efficient construction of generalized master equation memory kernels for multi-state systems from nonadiabatic quantum-classical dynamics.** *The Journal of chemical physics*
  Pfalzgraff, W. C., Montoya-Castillo, A. n., Kelly, A. n., Markland, T. E.
  2019; 150 (24): 244109
- **Hiding in the Crowd: Spectral Signatures of Overcoordinated Hydrogen-Bond Environments.** *The journal of physical chemistry letters*
  Morawietz, T. n., Urbina, A. S., Wise, P. K., Wu, X. n., Lu, W. n., Ben-Amotz, D. n., Markland, T. E.
  2019: 6067–73
- **Optical spectra in the condensed phase: Capturing anharmonic and vibronic features using dynamic and static approaches.** *The Journal of chemical physics*
  Zuehlsdorff, T. J., Montoya-Castillo, A. n., Napoli, J. A., Markland, T. E., Isborn, C. M.
  2019; 151 (7): 074111
- **Beyond Badger's Rule: The Origins and Generality of the Structure-Spectra Relationship of Aqueous Hydrogen Bonds.** *The journal of physical chemistry letters*
  Boyer, M. A., Marsalek, O. n., Heindel, J. P., Markland, T. E., McCoy, A. B., Xantheas, S. S.
  2019: 918–24
- **The Quest for Accurate Liquid Water Properties from First Principles** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
  Pestana, L., Marsalek, O., Markland, T. E., Head-Gordon, T.
  2018; 9 (17): 5009–16
- **On the exact continuous mapping of fermions.** *Scientific reports*
  Montoya-Castillo, A., Markland, T. E.
  2018; 8 (1): 12929
- **Unraveling electronic absorption spectra using nuclear quantum effects: Photoactive yellow protein and green fluorescent protein chromophores in water** *JOURNAL OF CHEMICAL PHYSICS*
  Zuehlsdorff, T. J., Napoli, J. A., Milanese, J. M., Markland, T. E., Isborn, C. M.
  2018; 149 (2): 024107
- **Decoding the spectroscopic features and time scales of aqueous proton defects.** *The Journal of chemical physics*

Napoli, J. A., Marsalek, O., Markland, T. E.
2018; 148 (22): 222833

- **Nuclear quantum effects enter the mainstream** *NATURE REVIEWS CHEMISTRY*
  Markland, T. E., Ceriotti, M.
  2018; 2 (3)
- **The Interplay of Structure and Dynamics in the Raman Spectrum of Liquid Water over the Full Frequency and Temperature Range** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
  Morawietz, T., Marsalek, O., Pattenaude, S. R., Streacker, L. M., Ben-Amotz, D., Markland, T. E.
  2018; 9 (4): 851–57
- **Proton Network Flexibility Enables Robustness and Large Electric Fields in the Ketosteroid Isomerase Active Site** *JOURNAL OF PHYSICAL CHEMISTRY B*
  Wang, L., Fried, S. D., Markland, T. E.
  2017; 121 (42): 9807–15
- **Unravelling the influence of quantum proton delocalization on electronic charge transfer through the hydrogen bond** *CHEMICAL PHYSICS LETTERS*
  Schran, C., Marsalek, O., Markland, T. E.
  2017; 678: 289–95
- **Quantum Dynamics and Spectroscopy of Ab Initio Liquid Water: The Interplay of Nuclear and Electronic Quantum Effects** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
  Marsalek, O., Markland, T. E.
  2017; 8 (7): 1545-1551
- **Electrostatic Control of Regioselectivity in Au(I)-Catalyzed Hydroarylation** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Lau, V. M., Pfalzgraff, W. C., Markland, T. E., Kanan, M. W.
  2017; 139 (11): 4035-4041
- **Nuclear Quantum Effects in Water and Aqueous Systems: Experiment, Theory, and Current Challenges** *CHEMICAL REVIEWS*
  Ceriotti, M., Fang, W., Kusalik, P. G., McKenzie, R. H., Michaelides, A., Morales, M. A., Markland, T. E.
  2016; 116 (13): 7529-7550
- **Generalized quantum master equations in and out of equilibrium: When can one win?** *JOURNAL OF CHEMICAL PHYSICS*
  Kelly, A., Montoya-Castillo, A., Wang, L., Markland, T. E.
  2016; 144 (18)
- **Unraveling the dynamics and structure of functionalized self-assembled monolayers on gold using 2D IR spectroscopy and MD simulations** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
  Yan, C., Yuan, R., Pfalzgraff, W. C., Nishida, J., Wang, L., Markland, T. E., Fayer, M. D.
  2016; 113 (18): 4929-4934
- **Ab initio molecular dynamics with nuclear quantum effects at classical cost: Ring polymer contraction for density functional theory** *JOURNAL OF CHEMICAL PHYSICS*
  Marsalek, O., Markland, T. E.
  2016; 144 (5)
- **Simulating Nuclear and Electronic Quantum Effects in Enzymes.** *Methods in enzymology*
  Wang, L., Isborn, C. M., Markland, T. E.
  2016; 577: 389-418
- **Nonadiabatic Dynamics in Atomistic Environments: Harnessing Quantum-Classical Theory with Generalized Quantum Master Equations** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
  Pfalzgraff, W. C., Kelly, A., Markland, T. E.
  2015; 6 (23): 4743-4748
- **Nonadiabatic Dynamics in Atomistic Environments: Harnessing Quantum-Classical Theory with Generalized Quantum Master Equations.** *The journal of physical chemistry letters*
  Pfalzgraff, W. C., Kelly, A., Markland, T. E.

2015; 6 (23): 4743-8

- **Accurate nonadiabatic quantum dynamics on the cheap: making the most of mean field theory with master equations.** *journal of chemical physics*
  Kelly, A., Brackbill, N., Markland, T. E.
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- **Accurate nonadiabatic quantum dynamics on the cheap: Making the most of mean field theory with master equations.** *journal of chemical physics*
  Kelly, A., Brackbill, N., Markland, T. E.
  2015; 142 (9): 094110-?
- **Quantum delocalization of protons in the hydrogen-bond network of an enzyme active site.** *Proceedings of the National Academy of Sciences of the United States of America*
  Wang, L., Fried, S. D., Boxer, S. G., Markland, T. E.
  2014; 111 (52): 18454-18459
- **Quantum fluctuations and isotope effects in ab initio descriptions of water** *JOURNAL OF CHEMICAL PHYSICS*
  Wang, L., Ceriotti, M., Markland, T. E.
  2014; 141 (10)
- **Quantum fluctuations and isotope effects in ab initio descriptions of water.** *journal of chemical physics*
  Wang, L., Ceriotti, M., Markland, T. E.
  2014; 141 (10): 104502-?
- **Multiple time step integrators in ab initio molecular dynamics.** *journal of chemical physics*
  Luehr, N., Markland, T. E., Martínez, T. J.
  2014; 140 (8): 084116-?
- **Interface-Limited Growth of Heterogeneously Nucleated Ice in Supercooled Water** *JOURNAL OF PHYSICAL CHEMISTRY B*
  Nistor, R. A., Markland, T. E., Berne, B. J.
  2014; 118 (3): 752-760
- **Efficient and accurate surface hopping for long time nonadiabatic quantum dynamics** *JOURNAL OF CHEMICAL PHYSICS*
  Kelly, A., Markland, T. E.
  2013; 139 (1)
- **Efficient methods and practical guidelines for simulating isotope effects** *JOURNAL OF CHEMICAL PHYSICS*
  Ceriotti, M., Markland, T. E.
  2013; 138 (1)
- **Ring-Polymer Molecular Dynamics: Quantum Effects in Chemical Dynamics from Classical Trajectories in an Extended Phase Space** *ANNUAL REVIEW OF PHYSICAL CHEMISTRY, VOL 64*
  Habershon, S., Manolopoulos, D. E., Markland, T. E., Miller, T. F.
  2013; 64: 387-413
- **Isotope effects in water as investigated by neutron diffraction and path integral molecular dynamics** *JOURNAL OF PHYSICS-CONDENSED MATTER*
  Zeidler, A., Salmon, P. S., Fischer, H. E., Neuefeind, J. C., Simonson, J. M., Markland, T. E.
  2012; 24 (28)
- **Zeidler et al. Reply** *PHYSICAL REVIEW LETTERS*
  Zeidler, A., Salmon, P. S., Fischer, H. E., Neuefeind, J. C., Simonson, J. M., Lemmel, H., Rauch, H., Markland, T. E.
  2012; 108 (25)
- **Growing Point-to-Set Length Scale Correlates with Growing Relaxation Times in Model Supercooled Liquids** *PHYSICAL REVIEW LETTERS*
  Hocky, G. M., Markland, T. E., Reichman, D. R.
  2012; 108 (22)
- **Unraveling quantum mechanical effects in water using isotopic fractionation** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*

Markland, T. E., Berne, B. J.
2012; 109 (21): 7988-7991

- **Reduced density matrix hybrid approach: Application to electronic energy transfer** *JOURNAL OF CHEMICAL PHYSICS*
  Berkelbach, T. C., Markland, T. E., Reichman, D. R.
  2012; 136 (8)
- **Theory and simulations of quantum glass forming liquids** *JOURNAL OF CHEMICAL PHYSICS*
  Markland, T. E., Morrone, J. A., Miyazaki, K., Berne, B. J., Reichman, D. R., Rabani, E.
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