Thomas E Markland

List of Publications by Year
in descending order

57 papers	4,689 citations	117571 34 h-index	143943 57 g-index
62 all docs	62 docs citations	62 times ranked	3656 citing authors

#	Article	IF	Citations
1	A two-directional vibrational probe reveals different electric field orientations in solution and an enzyme active site. Nature Chemistry, 2022, 14, 891-897.	6.6	33
2	Persistent Homology Metrics Reveal Quantum Fluctuations and Reactive Atoms in Path Integral Dynamics. Frontiers in Chemistry, 2021, 9, 624937.	1.8	2
3	AENETâ€“LAMMPS and AENETâ€“TINKER: Interfaces for accurate and efficient molecular dynamics simulations with machine learning potentials. Journal of Chemical Physics, 2021, 155, 074801.	1.2	12
4	Characterizing and Contrasting Structural Proton Transport Mechanisms in Azole Hydrogen Bond Networks Using Ab Initio Molecular Dynamics. Journal of Physical Chemistry Letters, 2021, 12, 8749-8756.	2.1	2
5	A framework for automated structure elucidation from routine NMR spectra. Chemical Science, 2021, 12, 15329-15338.	3.7	15
6	Exploiting Machine Learning to Efficiently Predict Multidimensional Optical Spectra in Complex Environments. Journal of Physical Chemistry Letters, 2020, 11, 7559-7568.	2.1	35
7	Resolving Heterogeneous Dynamics of Excess Protons in Aqueous Solution with Rate Theory. Journal of Physical Chemistry B, 2020, 124, 5665-5675.	1.2	17
8	Elucidating the Proton Transport Pathways in Liquid Imidazole with First-Principles Molecular Dynamics. Journal of Physical Chemistry Letters, 2020, 11, 6156-6163.	2.1	17
9	On the advantages of exploiting memory in Markov state models for biomolecular dynamics. Journal of Chemical Physics, 2020, 153, 014105.	1.2	37
10	Quantum kinetic energy and isotope fractionation in aqueous ionic solutions. Physical Chemistry Chemical Physics, 2020, 22, 10490-10499.	1.3	6
11	Excited state diabatization on the cheap using DFT: Photoinduced electron and hole transfer. Journal of Chemical Physics, 2020, 153, 244111.	1.2	13
12	Efficient construction of generalized master equation memory kernels for multi-state systems from nonadiabatic quantum-classical dynamics. Journal of Chemical Physics, 2019, 150, 244109.	1.2	33
13	Accurate and efficient DFT-based diabatization for hole and electron transfer using absolutely localized molecular orbitals. Journal of Chemical Physics, 2019, 151, 164114.	1.2	17
14	Optical spectra in the condensed phase: Capturing anharmonic and vibronic features using dynamic and static approaches. Journal of Chemical Physics, 2019, 151, 074111.	1.2	52
15	Hiding in the Crowd: Spectral Signatures of Overcoordinated Hydrogen-Bond Environments. Journal of Physical Chemistry Letters, 2019, 10, 6067-6073.	2.1	22
16	Tracking Aqueous Proton Transfer by Two-Dimensional Infrared Spectroscopy and ab Initio Molecular Dynamics Simulations. ACS Central Science, 2019, 5, 1269-1277.	5.3	47
17	Beyond Badgerâ€™s Rule: The Origins and Generality of the Structureâ€“Spectra Relationship of Aqueous Hydrogen Bonds. Journal of Physical Chemistry Letters, 2019, 10, 918-924.	2.1	52
18	i-PI 2.0: A universal force engine for advanced molecular simulations. Computer Physics Communications, 2019, 236, 214-223.	3.0	220

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19	Nuclear quantum effects enter the mainstream. Nature Reviews Chemistry, 2018, 2, .	13.8	271
20	Decoding the spectroscopic features and time scales of aqueous proton defects. Journal of Chemical Physics, 2018, 148, 222833.	1.2	33
21	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, 2018, 9, 851-857.	2.1	86
22	On the exact continuous mapping of fermions. Scientific Reports, 2018, 8, 12929.	1.6	4
23	Unraveling electronic absorption spectra using nuclear quantum effects: Photoactive yellow protein and green fluorescent protein chromophores in water. Journal of Chemical Physics, 2018, 149, 024107.	1.2	30
24	The Quest for Accurate Liquid Water Properties from First Principles. Journal of Physical Chemistry Letters, 2018, 9, 5009-5016.	2.1	70
25	Electrostatic Control of Regioselectivity in Au(I)-Catalyzed Hydroarylation. Journal of the American Chemical Society, 2017, 139, 4035-4041.	6.6	64
26	Unravelling the influence of quantum proton delocalization on electronic charge transfer through the hydrogen bond. Chemical Physics Letters, 2017, 678, 289-295.	1.2	30
27	Quantum Dynamics and Spectroscopy of Ab Initio Liquid Water: TheÂInterplay of Nuclear and Electronic Quantum Effects. Journal of Physical Chemistry Letters, 2017, 8, 1545-1551.	2.1	163
28	Proton Network Flexibility Enables Robustness and Large Electric Fields in the Ketosteroid Isomerase Active Site. Journal of Physical Chemistry B, 2017, 121, 9807-9815.	1.2	34
29	Ab initio molecular dynamics with nuclear quantum effects at classical cost: Ring polymer contraction for density functional theory. Journal of Chemical Physics, 2016, 144, 054112.	1.2	77
30	Generalized quantum master equations in and out of equilibrium: When can one win?. Journal of Chemical Physics, 2016, 144, 184105.	1.2	55
31	Nuclear Quantum Effects in Water and Aqueous Systems: Experiment, Theory, and Current Challenges. Chemical Reviews, 2016, 116, 7529-7550.	23.0	439
32	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, 2016, 113, 4929-4934.	3.3	48
33	Simulating Nuclear and Electronic Quantum Effects in Enzymes. Methods in Enzymology, 2016, 577, 389-418.	0.4	7
34	Accurate nonadiabatic quantum dynamics on the cheap: Making the most of mean field theory with master equations. Journal of Chemical Physics, 2015, 142, 094110.	1.2	52
35	Nonadiabatic Dynamics in Atomistic Environments: Harnessing Quantum-Classical Theory with Generalized Quantum Master Equations. Journal of Physical Chemistry Letters, 2015, 6, 4743-4748.	2.1	30
36	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, 2014, 111, 18454-18459.	3.3	115

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37	Quantum fluctuations and isotope effects in ab initio descriptions of water. Journal of Chemical Physics, 2014, 141, 104502.	1.2	68
38	Multiple time step integrators in ab initio molecular dynamics. Journal of Chemical Physics, 2014, 140, 084116.	1.2	33
39	Interface-Limited Growth of Heterogeneously Nucleated Ice in Supercooled Water. Journal of Physical Chemistry B, 2014, 118, 752-760.	1.2	29
40	Ring-Polymer Molecular Dynamics: Quantum Effects in Chemical Dynamics from Classical Trajectories in an Extended Phase Space. Annual Review of Physical Chemistry, 2013, 64, 387-413.	4.8	530
41	Efficient methods and practical guidelines for simulating isotope effects. Journal of Chemical Physics, 2013, 138, 014112.	1.2	78
42	Efficient and accurate surface hopping for long time nonadiabatic quantum dynamics. Journal of Chemical Physics, 2013, 139, 014104.	1.2	92
43	Unraveling quantum mechanical effects in water using isotopic fractionation. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 7988-7991.	3.3	97
44	Reduced density matrix hybrid approach: Application to electronic energy transfer. Journal of Chemical Physics, 2012, 136, 084104.	1.2	57
45	Reduced density matrix hybrid approach: An efficient and accurate method for adiabatic and non-adiabatic quantum dynamics. Journal of Chemical Physics, 2012, 136, 034113.	1.2	58
46	Isotope effects in water as investigated by neutron diffraction and path integral molecular dynamics. Journal of Physics Condensed Matter, 2012, 24, 284126.	0.7	47
47	Theory and simulations of quantum glass forming liquids. Journal of Chemical Physics, 2012, 136, 074511.	1.2	34
48	Growing Point-to-Set Length Scale Correlates with Growing Relaxation Times in Model Supercooled Liquids. Physical Review Letters, 2012, 108, 225506.	2.9	126
49	Efficient multiple time scale molecular dynamics: Using colored noise thermostats to stabilize resonances. Journal of Chemical Physics, 2011, 134, 014103.	1.2	61
50	Quantum fluctuations can promote or inhibit glassÂformation. Nature Physics, 2011, 7, 134-137.	6.5	84
51	Oxygen as a Site Specific Probe of the Structure of Water and Oxide Materials. Physical Review Letters, 2011, 107, 145501.	2.9	51
52	Efficient stochastic thermostatting of path integral molecular dynamics. Journal of Chemical Physics, 2010, 133, 124104.	1.2	259
53	A fast path integral method for polarizable force fields. Journal of Chemical Physics, 2009, 131, 094102.	1.2	41
54	Competing quantum effects in the dynamics of a flexible water model. Journal of Chemical Physics, 2009, 131, 024501.	1.2	426

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55	A refined ring polymer contraction scheme for systems with electrostatic interactions. Chemical Physics Letters, 2008, 464, 256-261.	1.2	70
56	Quantum diffusion of hydrogen and muonium atoms in liquid water and hexagonal ice. Journal of Chemical Physics, 2008, 128, 194506.	1.2	70
57	An efficient ring polymer contraction scheme for imaginary time path integral simulations. Journal of Chemical Physics, 2008, 129, 024105.	1.2	138