Thomas F Miller Iii

List of Publications by Year
in descending order

114 papers	6,891 citations	71004 43 h-index	71088 80 g-index
126 all docs	126 docs citations	126 times ranked	7063 citing authors

#	Article	IF	Citations
1	Equilibriumâ€“nonequilibrium ring-polymer molecular dynamics for nonlinear spectroscopy. Journal of Chemical Physics, 2022, 156, 131102.	1.2	7
2	Fast Near Ab Initio Potential Energy Surfaces Using Machine Learning. Journal of Physical Chemistry A, 2022, 126, 4013-4024.	1.1	10
3	Phosphine-Phenoxide Nickel Catalysts for Ethylene/Acrylate Copolymerization: Olefin Coordination and Complex Isomerization Studies Relevant to the Mechanism of Catalysis. Organometallics, 2022, 41, 2119-2131.	1.1	5
4	A generalized class of strongly stable and dimension-free T-RPMD integrators. Journal of Chemical Physics, 2021, 154, 024106.	1.2	6
5	Improved accuracy and transferability of molecular-orbital-based machine learning: Organics, transition-metal complexes, non-covalent interactions, and transition states. Journal of Chemical Physics, 2021, 154, 064108.	1.2	37
6	Residue-by-residue analysis of cotranslational membrane protein integration in vivo. ELife, 2021, 10, .	2.8	26
7	Small Nuclear Quantum Effects in Scattering of H and D from Graphene. Journal of Physical Chemistry Letters, 2021, 12, 1991-1996.	2.1	17
8	Interfacial Electron Transfer and Ion Solvation in the Solid Electrolyte Interphase. Journal of Physical Chemistry C, 2021, 125, 4614-4622.	1.5	6
9	Machine Learning Solvation Environments in Conductive Polymers: Application to ProDOT-2Hex with Solvent Swelling. Macromolecules, 2021, 54, 3377-3387.	2.2	10
10	Analytical gradients for molecular-orbital-based machine learning. Journal of Chemical Physics, 2021, 154, 124120.	1.2	9
11	Experimental and theoretical determinations of hydrogen isotopic equilibrium in the system CH4H2H2O from 3 to 200â€Â°C. Geochimica Et Cosmochimica Acta, 2021, 314, 223-269.	1.6	23
12	Efficient Copolymerization of Acrylate and Ethylene with Neutral P, O-Chelated Nickel Catalysts: Mechanistic Investigations of Monomer Insertion and Chelate Formation. Journal of the American Chemical Society, 2021, 143, 6516-6527.	6.6	49
13	Force transduction creates long-ranged coupling in ribosomes stalled by arrest peptides. Biophysical Journal, 2021, 120, 2425-2435.	0.2	11
14	A New Imaginary Term in the Second-Order Nonlinear Susceptibility from Charged Interfaces. Journal of Physical Chemistry Letters, 2021, 12, 5649-5659.	2.1	32
15	Electronic Structure of Superoxidized Radical Cationic Dodecaborate-Based Clusters. Journal of Physical Chemistry A, 2021, 125, 6141-6150.	1.1	2
16	Stern and Diffuse Layer Interactions during Ionic Strength Cycling. Journal of Physical Chemistry C, 2021, 125, 18002-18014.	1.5	20
17	Li+ and Oxidant Addition To Control Ionic and Electronic Conduction in Ionic Liquid-Functionalized Conjugated Polymers. Chemistry of Materials, 2021, 33, 6464-6474.	3.2	13
18	OrbNet Denali: A machine learning potential for biological and organic chemistry with semi-empirical cost and DFT accuracy. Journal of Chemical Physics, 2021, 155, 204103.	1.2	40

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19	Coordination of -1 programmed ribosomal frameshifting by transcript and nascent chain features revealed by deep mutational scanning. Nucleic Acids Research, 2021, 49, 12943-12954.	6.5	12
20	OrbNet: Deep learning for quantum chemistry using symmetry-adapted atomic-orbital features. Journal of Chemical Physics, 2020, 153, 124111.	1.2	153
21	Dihexyl-Substituted Poly(3,4-Propylenedioxythiophene) as a Dual Ionic and Electronic Conductive Cathode Binder for Lithium-Ion Batteries. Chemistry of Materials, 2020, 32, 9176-9189.	3.2	42
22	Sum-Frequency Signals in 2D-Terahertz-Terahertz-Raman Spectroscopy. Journal of Physical Chemistry B, 2020, 124, 8904-8908.	1.2	15
23	Electronically Modified Cobalt Aminopyridine Complexes Reveal an Orthogonal Axis for Catalytic Optimization for CO₂ Reduction. Inorganic Chemistry, 2020, 59, 13709-13718.	1.9	11
24	The Journal of Physical Chemistry A/B/C Virtual Special Issue on Machine Learning in Physical Chemistry. Journal of Physical Chemistry B, 2020, 124, 9767-9772.	1.2	2
25	The Journal of Physical Chemistry A/B/C Virtual Special Issue on Machine Learning in Physical Chemistry. Journal of Physical Chemistry A, 2020, 124, 9113-9118.	1.1	2
26	The Journal of Physical Chemistry A/B/C Virtual Special Issue on Machine Learning in Physical Chemistry. Journal of Physical Chemistry C, 2020, 124, 24033-24038.	1.5	1
27	Dimension-free path-integral molecular dynamics without preconditioning. Journal of Chemical Physics, 2020, 152, 104102.	1.2	19
28	Dynamics of Co-translational Membrane Protein Integration and Translocation via the Sec Translocon. Journal of the American Chemical Society, 2020, 142, 5449-5460.	6.6	8
29	Cotranslational folding stimulates programmed ribosomal frameshifting in the alphavirus structural polyprotein. Journal of Biological Chemistry, 2020, 295, 6798-6808.	1.6	32
30	Microcanonical rates from ring-polymer molecular dynamics: Direct-shooting, stationary-phase, and maximum-entropy approaches. Journal of Chemical Physics, 2020, 152, 124117.	1.2	16
31	A Super-Oxidized Radical Cationic Icosahedral Boron Cluster. Journal of the American Chemical Society, 2020, 142, 12948-12953.	6.6	16
32	The Molpro quantum chemistry package. Journal of Chemical Physics, 2020, 152, 144107.	1.2	603
33	Embedded Mean-Field Theory for Solution-Phase Transition-Metal Polyolefin Catalysis. Journal of Chemical Theory and Computation, 2020, 16, 4226-4237.	2.3	3
34	Analytical gradients for projection-based wavefunction-in-DFT embedding. Journal of Chemical Physics, 2019, 151, .	1.2	17
35	Energy conversion via metal nanolayers. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 16210-16215.	3.3	26
36	Interpretation of the THz-THz-Raman Spectrum of Bromoform. Journal of Physical Chemistry A, 2019, 123, 7278-7287.	1.1	10

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37	Regression Clustering for Improved Accuracy and Training Costs with Molecular-Orbital-Based Machine Learning. Journal of Chemical Theory and Computation, 2019, 15, 6668-6677.	2.3	49
38	Path-accelerated stochastic molecular dynamics: Parallel-in-time integration using path integrals. Journal of Chemical Physics, 2019, 151, 164120.	1.2	3
39	Real-time density-matrix coupled-cluster approach for closed and open systems at finite temperature. Journal of Chemical Physics, 2019, 151, 134107.	1.2	20
40	Cayley modification for strongly stable path-integral and ring-polymer molecular dynamics. Journal of Chemical Physics, 2019, 151, 124103.	1.2	25
41	Direct dioxygen evolution in collisions of carbon dioxide with surfaces. Nature Communications, 2019, 10, 2294.	5.8	16
42	Imaging covalent bond formation by H atom scattering from graphene. Science, 2019, 364, 379-382.	6.0	76
43	Projection-Based Wavefunction-in-DFT Embedding. Accounts of Chemical Research, 2019, 52, 1359-1368.	7.6	88
44	A universal density matrix functional from molecular orbital-based machine learning: Transferability across organic molecules. Journal of Chemical Physics, 2019, 150, 131103.	1.2	88
45	Simple Flux-Side Formulation of State-Resolved Thermal Reaction Rates for Ring-Polymer Surface Hopping. Journal of Physical Chemistry A, 2019, 123, 3013-3020.	1.1	21
46	Fluoride-ion solvation in non-aqueous electrolyte solutions. Materials Chemistry Frontiers, 2019, 3, 2721-2727.	3.2	12
47	Comparison of Experimental vs Theoretical Abundances of ¹³CH₃D and ¹²CH₂D₂ for Isotopically Equilibrated Systems from 1 to 500 Â°C. ACS Earth and Space Chemistry, 2019, 3, 2747-2764.	1.2	41
48	Pendant Hydrogen-Bond Donors in Cobalt Catalysts Independently Enhance CO₂ Reduction. ACS Central Science, 2018, 4, 397-404.	5.3	163
49	Optimizing Ion Transport in Polyether-Based Electrolytes for Lithium Batteries. Macromolecules, 2018, 51, 2847-2858.	2.2	86
50	Path-integral isomorphic Hamiltonian for including nuclear quantum effects in non-adiabatic dynamics. Journal of Chemical Physics, 2018, 148, 102327.	1.2	45
51	Room-temperature cycling of metal fluoride electrodes: Liquid electrolytes for high-energy fluoride ion cells. Science, 2018, 362, 1144-1148.	6.0	157
52	Forces on Nascent Polypeptides during Membrane Insertion and Translocation via the Sec Translocon. Biophysical Journal, 2018, 115, 1885-1894.	0.2	30
53	Even-handed subsystem selection in projection-based embedding. Journal of Chemical Physics, 2018, 149, 144101.	1.2	36
54	Fluctuating hydrogen-bond networks govern anomalous electron transfer kinetics in a blue copper protein. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 6129-6134.	3.3	34

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55	Transferability in Machine Learning for Electronic Structure via the Molecular Orbital Basis. Journal of Chemical Theory and Computation, 2018, 14, 4772-4779.	2.3	149
56	Globally Suppressed Dynamics in Ion-Doped Polymers. ACS Macro Letters, 2018, 7, 734-738.	2.3	20
57	Enhancing Cation Diffusion and Suppressing Anion Diffusion via Lewis-Acidic Polymer Electrolytes. Journal of Physical Chemistry Letters, 2017, 8, 641-646.	2.1	105
58	Correcting density-driven errors in projection-based embedding. Journal of Chemical Physics, 2017, 146, 084113.	1.2	14
59	Density-based errors in mixed-basis mean-field electronic structure, with implications for embedding and QM/MM methods. Chemical Physics Letters, 2017, 683, 375-382.	1.2	4
60	Embedded Mean-Field Theory with Block-Orthogonalized Partitioning. Journal of Chemical Theory and Computation, 2017, 13, 1605-1615.	2.3	35
61	Designing Polymer Electrolytes for Safe and High Capacity Rechargeable Lithium Batteries. Accounts of Chemical Research, 2017, 50, 590-593.	7.6	149
62	Improving membrane protein expression by optimizing integration efficiency. Journal of Biological Chemistry, 2017, 292, 19537-19545.	1.6	13
63	2D THz-THz-Raman Photon-Echo Spectroscopy of Molecular Vibrations in Liquid Bromoform. Journal of Physical Chemistry Letters, 2017, 8, 4640-4644.	2.1	39
64	Linear-Response Time-Dependent Embedded Mean-Field Theory. Journal of Chemical Theory and Computation, 2017, 13, 4216-4227.	2.3	20
65	Equilibrium clumped-isotope effects in doubly substituted isotopologues of ethane. Geochimica Et Cosmochimica Acta, 2017, 197, 14-26.	1.6	15
66	Two-step membrane binding by the bacterial SRP receptor enable efficient and accurate Co-translational protein targeting. ELife, 2017, 6, .	2.8	7
67	Structurally detailed coarse-grained model for Sec-facilitated co-translational protein translocation and membrane integration. PLoS Computational Biology, 2017, 13, e1005427.	1.5	22
68	Non-equilibrium dynamics from RPMD and CMD. Journal of Chemical Physics, 2016, 145, 204118.	1.2	48
69	Kinetically-constrained ring-polymer molecular dynamics for non-adiabatic chemistries involving solvent and donorâ€“acceptor dynamical effects. Faraday Discussions, 2016, 195, 191-214.	1.6	23
70	Breaking the Correlation between Energy Costs and Kinetic Barriers in Hydrogen Evolution via a Cobalt Pyridine-Diimine-Dioxime Catalyst. ACS Catalysis, 2016, 6, 6114-6123.	5.5	51
71	Molecular Seesaw: How Increased Hydrogen Bonding Can Hinder Excited-State Proton Transfer. Journal of Physical Chemistry Letters, 2016, 7, 3616-3620.	2.1	14
72	A Link between Integral Membrane Protein Expression and Simulated Integration Efficiency. Cell Reports, 2016, 16, 2169-2177.	2.9	17

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73	Universal Relationship between Conductivity and Solvation-Site Connectivity in Ether-Based Polymer Electrolytes. Macromolecules, 2016, 49, 5244-5255.	2.2	66
74	Fock-Matrix Corrections in Density Functional Theory and Use in Embedded Mean-Field Theory. Journal of Chemical Theory and Computation, 2016, 12, 5811-5822.	2.3	15
75	Coherent two-dimensional terahertz-terahertz-Raman spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 6857-6861.	3.3	80
76	Effect of monomer structure on ionic conductivity in a systematic set of polyester electrolytes. Solid State Ionics, 2016, 289, 118-124.	1.3	62
77	Tipping the Balance between Concerted versus Sequential Proton-Coupled Electron Transfer. Inorganic Chemistry, 2016, 55, 1022-1031.	1.9	35
78	Embedded Mean-Field Theory. Journal of Chemical Theory and Computation, 2015, 11, 568-580.	2.3	83
79	Ab Initio Characterization of the Electrochemical Stability and Solvation Properties of Condensed-Phase Ethylene Carbonate and Dimethyl Carbonate Mixtures. Journal of Physical Chemistry C, 2015, 119, 3865-3880.	1.5	50
80	Systematic Computational and Experimental Investigation of Lithium-Ion Transport Mechanisms in Polyester-Based Polymer Electrolytes. ACS Central Science, 2015, 1, 198-205.	5.3	162
81	Chemically Specific Dynamic Bond Percolation Model for Ion Transport in Polymer Electrolytes. Macromolecules, 2015, 48, 7346-7358.	2.2	77
82	Nuclear Quantum Effects in the Layering and Diffusion of Hydrogen Isotopes in Carbon Nanotubes. Journal of Physical Chemistry Letters, 2015, 6, 3367-3372.	2.1	15
83	Electronic coherence and the kinetics of inter-complex energy transfer in light-harvesting systems. Physical Chemistry Chemical Physics, 2015, 17, 30914-30924.	1.3	12
84	Accelerating wavefunction in density-functional-theory embedding by truncating the active basis set. Journal of Chemical Physics, 2015, 143, 024105.	1.2	60
85	Regulation of multispanning membrane protein topology via post-translational annealing. ELife, 2015, 4, .	2.8	42
86	Allosteric Response and Substrate Sensitivity in Peptide Binding of the Signal Recognition Particle. Journal of Biological Chemistry, 2014, 289, 30868-30879.	1.6	2
87	Kinetically constrained ring-polymer molecular dynamics for non-adiabatic chemical reactions. Journal of Chemical Physics, 2014, 140, 064103.	1.2	89
88	Accurate and systematically improvable density functional theory embedding for correlated wavefunctions. Journal of Chemical Physics, 2014, 140, 18A507.	1.2	127
89	Position-Specific and Clumped Stable Isotope Studies: Comparison of the Urey and Path-Integral Approaches for Carbon Dioxide, Nitrous Oxide, Methane, and Propane. Journal of Physical Chemistry A, 2014, 118, 467-474.	1.1	88
90	Direct simulation of proton-coupled electron transfer across multiple regimes. Journal of Chemical Physics, 2013, 138, 134109.	1.2	74

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91	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
92	Accurate basis set truncation for wavefunction embedding. Journal of Chemical Physics, 2013, 139, 024103.	1.2	79
93	Communication: Predictive partial linearized path integral simulation of condensed phase electron transfer dynamics. Journal of Chemical Physics, 2013, 139, 151103.	1.2	64
94	Density functional theory embedding for correlated wavefunctions: Improved methods for open-shell systems and transition metal complexes. Journal of Chemical Physics, 2012, 137, 224113.	1.2	104
95	Long-Timescale Dynamics and Regulation of Sec-Facilitated Protein Translocation. Cell Reports, 2012, 2, 927-937.	2.9	52
96	Flux-correlation approach to characterizing reaction pathways in quantum systems: a study of condensed-phase proton-coupled electron transfer. Molecular Physics, 2012, 110, 1009-1015.	0.8	17
97	Direct Simulation of Early-Stage Sec-Facilitated Protein Translocation. Journal of the American Chemical Society, 2012, 134, 13700-13707.	6.6	26
98	Suppression of Dendrite Formation via Pulse Charging in Rechargeable Lithium Metal Batteries. Journal of Physical Chemistry C, 2012, 116, 26214-26221.	1.5	165
99	A Simple, Exact Density-Functional-Theory Embedding Scheme. Journal of Chemical Theory and Computation, 2012, 8, 2564-2568.	2.3	299
100	Direct simulation of electron transfer using ring polymer molecular dynamics: Comparison with semiclassical instanton theory and exact quantum methods. Journal of Chemical Physics, 2011, 135, 074106.	1.2	105
101	Dynamics and dissipation in enzyme catalysis. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 16159-16163.	3.3	141
102	Embedded density functional theory for covalently bonded and strongly interacting subsystems. Journal of Chemical Physics, 2011, 134, 164108.	1.2	87
103	Exact nonadditive kinetic potentials for embedded density functional theory. Journal of Chemical Physics, 2010, 133, 084103.	1.2	171
104	Exact quantum statistics for electronically nonadiabatic systems using continuous path variables. Journal of Chemical Physics, 2010, 133, 234103.	1.2	71
105	Hydrophobically stabilized open state for the lateral gate of the Sec translocon. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 5399-5404.	3.3	54
106	Ring polymer molecular dynamics beyond the linear response regime: Excess electron injection and trapping in liquids. Journal of Chemical Physics, 2010, 132, 034106.	1.2	35
107	Isomorphic classical molecular dynamics model for an excess electron in a supercritical fluid. Journal of Chemical Physics, 2008, 129, 194502.	1.2	42
108	Sampling diffusive transition paths. Journal of Chemical Physics, 2007, 126, 144102.	1.2	25

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109	Solvent coarse-graining and the string method applied to the hydrophobic collapse of a hydrated chain. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 14559-14564.	3.3	155
110	Quantum Simulation of a Hydrated Noradrenaline Analog with the Torsional Path Integral Methodâ€. Journal of Physical Chemistry A, 2006, 110, 731-740.	1.1	13
111	Quantum diffusion in liquid para-hydrogen from ring-polymer molecular dynamics. Journal of Chemical Physics, 2005, 122, 184503.	1.2	142
112	Quantum diffusion in liquid water from ring polymer molecular dynamics. Journal of Chemical Physics, 2005, 123, 154504.	1.2	182
113	Quantum free energies of the conformers of glycine on an ab initio potential energy surfaceElectronic supplementary information (ESI) available: Calculated harmonic frequencies of the glycine conformers. See http://www.rsc.org/suppdata/cp/b3/b314644h/. Physical Chemistry Chemical Physics, 2004, 6, 2563.	1.3	55
114	Torsional path integral Monte Carlo method for calculating the absolute quantum free energy of large molecules. Journal of Chemical Physics, 2003, 119, 68-76.	1.2	36