Thomas F Miller Iii

List of Publications by Year
in descending order

114 papers	6,891 citations	61984 43 h-index	62596 80 g-index
126 all docs	126 docs citations	126 times ranked	6127 citing authors

#	Article	IF	Citations
1	The Molpro quantum chemistry package. Journal of Chemical Physics, 2020, 152, 144107.	3.0	603
2	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.	10.8	530
3	A Simple, Exact Density-Functional-Theory Embedding Scheme. Journal of Chemical Theory and Computation, 2012, 8, 2564-2568.	5.3	299
4	Quantum diffusion in liquid water from ring polymer molecular dynamics. Journal of Chemical Physics, 2005, 123, 154504.	3.0	182
5	Exact nonadditive kinetic potentials for embedded density functional theory. Journal of Chemical Physics, 2010, 133, 084103.	3.0	171
6	Suppression of Dendrite Formation via Pulse Charging in Rechargeable Lithium Metal Batteries. Journal of Physical Chemistry C, 2012, 116, 26214-26221.	3.1	165
7	Pendant Hydrogen-Bond Donors in Cobalt Catalysts Independently Enhance CO₂ Reduction. ACS Central Science, 2018, 4, 397-404.	11.3	163
8	Systematic Computational and Experimental Investigation of Lithium-Ion Transport Mechanisms in Polyester-Based Polymer Electrolytes. ACS Central Science, 2015, 1, 198-205.	11.3	162
9	Room-temperature cycling of metal fluoride electrodes: Liquid electrolytes for high-energy fluoride ion cells. Science, 2018, 362, 1144-1148.	12.6	157
10	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.	7.1	155
11	OrbNet: Deep learning for quantum chemistry using symmetry-adapted atomic-orbital features. Journal of Chemical Physics, 2020, 153, 124111.	3.0	153
12	Designing Polymer Electrolytes for Safe and High Capacity Rechargeable Lithium Batteries. Accounts of Chemical Research, 2017, 50, 590-593.	15.6	149
13	Transferability in Machine Learning for Electronic Structure via the Molecular Orbital Basis. Journal of Chemical Theory and Computation, 2018, 14, 4772-4779.	5.3	149
14	Quantum diffusion in liquid para-hydrogen from ring-polymer molecular dynamics. Journal of Chemical Physics, 2005, 122, 184503.	3.0	142
15	Dynamics and dissipation in enzyme catalysis. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 16159-16163.	7.1	141
16	Accurate and systematically improvable density functional theory embedding for correlated wavefunctions. Journal of Chemical Physics, 2014, 140, 18A507.	3.0	127
17	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.	3.0	105
18	Enhancing Cation Diffusion and Suppressing Anion Diffusion via Lewis-Acidic Polymer Electrolytes. Journal of Physical Chemistry Letters, 2017, 8, 641-646.	4.6	105

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19	Density functional theory embedding for correlated wavefunctions: Improved methods for open-shell systems and transition metal complexes. Journal of Chemical Physics, 2012, 137, 224113.	3.0	104
20	Kinetically constrained ring-polymer molecular dynamics for non-adiabatic chemical reactions. Journal of Chemical Physics, 2014, 140, 064103.	3.0	89
21	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.	2.5	88
22	Projection-Based Wavefunction-in-DFT Embedding. Accounts of Chemical Research, 2019, 52, 1359-1368.	15.6	88
23	A universal density matrix functional from molecular orbital-based machine learning: Transferability across organic molecules. Journal of Chemical Physics, 2019, 150, 131103.	3.0	88
24	Embedded density functional theory for covalently bonded and strongly interacting subsystems. Journal of Chemical Physics, 2011, 134, 164108.	3.0	87
25	Optimizing Ion Transport in Polyether-Based Electrolytes for Lithium Batteries. Macromolecules, 2018, 51, 2847-2858.	4.8	86
26	Embedded Mean-Field Theory. Journal of Chemical Theory and Computation, 2015, 11, 568-580.	5.3	83
27	Coherent two-dimensional terahertz-terahertz-Raman spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 6857-6861.	7.1	80
28	Accurate basis set truncation for wavefunction embedding. Journal of Chemical Physics, 2013, 139, 024103.	3.0	79
29	Chemically Specific Dynamic Bond Percolation Model for Ion Transport in Polymer Electrolytes. Macromolecules, 2015, 48, 7346-7358.	4.8	77
30	Imaging covalent bond formation by H atom scattering from graphene. Science, 2019, 364, 379-382.	12.6	76
31	Direct simulation of proton-coupled electron transfer across multiple regimes. Journal of Chemical Physics, 2013, 138, 134109.	3.0	74
32	Exact quantum statistics for electronically nonadiabatic systems using continuous path variables. Journal of Chemical Physics, 2010, 133, 234103.	3.0	71
33	Universal Relationship between Conductivity and Solvation-Site Connectivity in Ether-Based Polymer Electrolytes. Macromolecules, 2016, 49, 5244-5255.	4.8	66
34	Communication: Predictive partial linearized path integral simulation of condensed phase electron transfer dynamics. Journal of Chemical Physics, 2013, 139, 151103.	3.0	64
35	Effect of monomer structure on ionic conductivity in a systematic set of polyester electrolytes. Solid State Ionics, 2016, 289, 118-124.	2.7	62
36	Accelerating wavefunction in density-functional-theory embedding by truncating the active basis set. Journal of Chemical Physics, 2015, 143, 024105.	3.0	60

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37	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.	2.8	55
38	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.	7.1	54
39	Long-Timescale Dynamics and Regulation of Sec-Facilitated Protein Translocation. Cell Reports, 2012, 2, 927-937.	6.4	52
40	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.	11.2	51
41	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.	3.1	50
42	Regression Clustering for Improved Accuracy and Training Costs with Molecular-Orbital-Based Machine Learning. Journal of Chemical Theory and Computation, 2019, 15, 6668-6677.	5.3	49
43	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.	13.7	49
44	Non-equilibrium dynamics from RPMD and CMD. Journal of Chemical Physics, 2016, 145, 204118.	3.0	48
45	Path-integral isomorphic Hamiltonian for including nuclear quantum effects in non-adiabatic dynamics. Journal of Chemical Physics, 2018, 148, 102327.	3.0	45
46	Isomorphic classical molecular dynamics model for an excess electron in a supercritical fluid. Journal of Chemical Physics, 2008, 129, 194502.	3.0	42
47	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.	6.7	42
48	Regulation of multispanning membrane protein topology via post-translational annealing. ELife, 2015, 4, .	6.0	42
49	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.	2.7	41
50	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.	3.0	40
51	2D THz-THz-Raman Photon-Echo Spectroscopy of Molecular Vibrations in Liquid Bromoform. Journal of Physical Chemistry Letters, 2017, 8, 4640-4644.	4.6	39
52	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.	3.0	37
53	Torsional path integral Monte Carlo method for calculating the absolute quantum free energy of large molecules. Journal of Chemical Physics, 2003, 119, 68-76.	3.0	36
54	Even-handed subsystem selection in projection-based embedding. Journal of Chemical Physics, 2018, 149, 144101.	3.0	36

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55	Ring polymer molecular dynamics beyond the linear response regime: Excess electron injection and trapping in liquids. Journal of Chemical Physics, 2010, 132, 034106.	3.0	35
56	Tipping the Balance between Concerted versus Sequential Proton-Coupled Electron Transfer. Inorganic Chemistry, 2016, 55, 1022-1031.	4.0	35
57	Embedded Mean-Field Theory with Block-Orthogonalized Partitioning. Journal of Chemical Theory and Computation, 2017, 13, 1605-1615.	5.3	35
58	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.	7.1	34
59	Cotranslational folding stimulates programmed ribosomal frameshifting in the alphavirus structural polyprotein. Journal of Biological Chemistry, 2020, 295, 6798-6808.	3.4	32
60	A New Imaginary Term in the Second-Order Nonlinear Susceptibility from Charged Interfaces. Journal of Physical Chemistry Letters, 2021, 12, 5649-5659.	4.6	32
61	Forces on Nascent Polypeptides during Membrane Insertion and Translocation via the Sec Translocon. Biophysical Journal, 2018, 115, 1885-1894.	0.5	30
62	Direct Simulation of Early-Stage Sec-Facilitated Protein Translocation. Journal of the American Chemical Society, 2012, 134, 13700-13707.	13.7	26
63	Energy conversion via metal nanolayers. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 16210-16215.	7.1	26
64	Residue-by-residue analysis of cotranslational membrane protein integration in vivo. ELife, 2021, 10, .	6.0	26
65	Sampling diffusive transition paths. Journal of Chemical Physics, 2007, 126, 144102.	3.0	25
66	Cayley modification for strongly stable path-integral and ring-polymer molecular dynamics. Journal of Chemical Physics, 2019, 151, 124103.	3.0	25
67	Kinetically-constrained ring-polymer molecular dynamics for non-adiabatic chemistries involving solvent and donorâ€“acceptor dynamical effects. Faraday Discussions, 2016, 195, 191-214.	3.2	23
68	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.	3.9	23
69	Structurally detailed coarse-grained model for Sec-facilitated co-translational protein translocation and membrane integration. PLoS Computational Biology, 2017, 13, e1005427.	3.2	22
70	Simple Flux-Side Formulation of State-Resolved Thermal Reaction Rates for Ring-Polymer Surface Hopping. Journal of Physical Chemistry A, 2019, 123, 3013-3020.	2.5	21
71	Linear-Response Time-Dependent Embedded Mean-Field Theory. Journal of Chemical Theory and Computation, 2017, 13, 4216-4227.	5.3	20
72	Globally Suppressed Dynamics in Ion-Doped Polymers. ACS Macro Letters, 2018, 7, 734-738.	4.8	20

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73	Real-time density-matrix coupled-cluster approach for closed and open systems at finite temperature. Journal of Chemical Physics, 2019, 151, 134107.	3.0	20
74	Stern and Diffuse Layer Interactions during Ionic Strength Cycling. Journal of Physical Chemistry C, 2021, 125, 18002-18014.	3.1	20
75	Dimension-free path-integral molecular dynamics without preconditioning. Journal of Chemical Physics, 2020, 152, 104102.	3.0	19
76	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.	1.7	17
77	A Link between Integral Membrane Protein Expression and Simulated Integration Efficiency. Cell Reports, 2016, 16, 2169-2177.	6.4	17
78	Analytical gradients for projection-based wavefunction-in-DFT embedding. Journal of Chemical Physics, 2019, 151, .	3.0	17
79	Small Nuclear Quantum Effects in Scattering of H and D from Graphene. Journal of Physical Chemistry Letters, 2021, 12, 1991-1996.	4.6	17
80	Direct dioxygen evolution in collisions of carbon dioxide with surfaces. Nature Communications, 2019, 10, 2294.	12.8	16
81	Microcanonical rates from ring-polymer molecular dynamics: Direct-shooting, stationary-phase, and maximum-entropy approaches. Journal of Chemical Physics, 2020, 152, 124117.	3.0	16
82	A Super-Oxidized Radical Cationic Icosahedral Boron Cluster. Journal of the American Chemical Society, 2020, 142, 12948-12953.	13.7	16
83	Nuclear Quantum Effects in the Layering and Diffusion of Hydrogen Isotopes in Carbon Nanotubes. Journal of Physical Chemistry Letters, 2015, 6, 3367-3372.	4.6	15
84	Fock-Matrix Corrections in Density Functional Theory and Use in Embedded Mean-Field Theory. Journal of Chemical Theory and Computation, 2016, 12, 5811-5822.	5.3	15
85	Equilibrium clumped-isotope effects in doubly substituted isotopologues of ethane. Geochimica Et Cosmochimica Acta, 2017, 197, 14-26.	3.9	15
86	Sum-Frequency Signals in 2D-Terahertz-Terahertz-Raman Spectroscopy. Journal of Physical Chemistry B, 2020, 124, 8904-8908.	2.6	15
87	Molecular Seesaw: How Increased Hydrogen Bonding Can Hinder Excited-State Proton Transfer. Journal of Physical Chemistry Letters, 2016, 7, 3616-3620.	4.6	14
88	Correcting density-driven errors in projection-based embedding. Journal of Chemical Physics, 2017, 146, 084113.	3.0	14
89	Quantum Simulation of a Hydrated Noradrenaline Analog with the Torsional Path Integral Methodâ€. Journal of Physical Chemistry A, 2006, 110, 731-740.	2.5	13
90	Improving membrane protein expression by optimizing integration efficiency. Journal of Biological Chemistry, 2017, 292, 19537-19545.	3.4	13

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91	Li+ and Oxidant Addition To Control Ionic and Electronic Conduction in Ionic Liquid-Functionalized Conjugated Polymers. Chemistry of Materials, 2021, 33, 6464-6474.	6.7	13
92	Electronic coherence and the kinetics of inter-complex energy transfer in light-harvesting systems. Physical Chemistry Chemical Physics, 2015, 17, 30914-30924.	2.8	12
93	Fluoride-ion solvation in non-aqueous electrolyte solutions. Materials Chemistry Frontiers, 2019, 3, 2721-2727.	5.9	12
94	Coordination of -1 programmed ribosomal frameshifting by transcript and nascent chain features revealed by deep mutational scanning. Nucleic Acids Research, 2021, 49, 12943-12954.	14.5	12
95	Electronically Modified Cobalt Aminopyridine Complexes Reveal an Orthogonal Axis for Catalytic Optimization for CO₂ Reduction. Inorganic Chemistry, 2020, 59, 13709-13718.	4.0	11
96	Force transduction creates long-ranged coupling in ribosomes stalled by arrest peptides. Biophysical Journal, 2021, 120, 2425-2435.	0.5	11
97	Interpretation of the THz-THz-Raman Spectrum of Bromoform. Journal of Physical Chemistry A, 2019, 123, 7278-7287.	2.5	10
98	Machine Learning Solvation Environments in Conductive Polymers: Application to ProDOT-2Hex with Solvent Swelling. Macromolecules, 2021, 54, 3377-3387.	4.8	10
99	Fast Near Ab Initio Potential Energy Surfaces Using Machine Learning. Journal of Physical Chemistry A, 2022, 126, 4013-4024.	2.5	10
100	Analytical gradients for molecular-orbital-based machine learning. Journal of Chemical Physics, 2021, 154, 124120.	3.0	9
101	Dynamics of Co-translational Membrane Protein Integration and Translocation via the Sec Translocon. Journal of the American Chemical Society, 2020, 142, 5449-5460.	13.7	8
102	Two-step membrane binding by the bacterial SRP receptor enable efficient and accurate Co-translational protein targeting. ELife, 2017, 6, .	6.0	7
103	Equilibriumâ€“nonequilibrium ring-polymer molecular dynamics for nonlinear spectroscopy. Journal of Chemical Physics, 2022, 156, 131102.	3.0	7
104	A generalized class of strongly stable and dimension-free T-RPMD integrators. Journal of Chemical Physics, 2021, 154, 024106.	3.0	6
105	Interfacial Electron Transfer and Ion Solvation in the Solid Electrolyte Interphase. Journal of Physical Chemistry C, 2021, 125, 4614-4622.	3.1	6
106	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.	2.3	5
107	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.	2.6	4
108	Path-accelerated stochastic molecular dynamics: Parallel-in-time integration using path integrals. Journal of Chemical Physics, 2019, 151, 164120.	3.0	3

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109	Embedded Mean-Field Theory for Solution-Phase Transition-Metal Polyolefin Catalysis. Journal of Chemical Theory and Computation, 2020, 16, 4226-4237.	5.3	3
110	Allosteric Response and Substrate Sensitivity in Peptide Binding of the Signal Recognition Particle. Journal of Biological Chemistry, 2014, 289, 30868-30879.	3.4	2
111	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.	2.6	2
112	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.	2.5	2
113	Electronic Structure of Superoxidized Radical Cationic Dodecaborate-Based Clusters. Journal of Physical Chemistry A, 2021, 125, 6141-6150.	2.5	2
114	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.	3.1	1