Dan Mendels

List of Publications by Year
in descending order

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72	28,824	94433 37	82547 72
papers	citations	h-index	g-index

73	73	73	26185
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Canonical sampling through velocity rescaling. Journal of Chemical Physics, 2007, 126, 014101.	3.0	11,867
2	Escaping free-energy minima. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 12562-12566.	7.1	4,527
3	Quickstep: Fast and accurate density functional calculations using a mixed Gaussian and plane waves approach. Computer Physics Communications, 2005, 167, 103-128.	7.5	4,200
4	Well-Tempered Metadynamics: A Smoothly Converging and Tunable Free-Energy Method. Physical Review Letters, 2008, 100, 020603.	7.8	2,201
5	Enhancing Important Fluctuations: Rare Events and Metadynamics from a Conceptual Viewpoint. Annual Review of Physical Chemistry, 2016, 67, 159-184.	10.8	497
6	From A to B in free energy space. Journal of Chemical Physics, 2007, 126, 054103.	3.0	476
7	Free-Energy Landscape for Î² Hairpin Folding from Combined Parallel Tempering and Metadynamics. Journal of the American Chemical Society, 2006, 128, 13435-13441.	13.7	458
8	A Time-Independent Free Energy Estimator for Metadynamics. Journal of Physical Chemistry B, 2015, 119, 736-742.	2.6	399
9	Funnel metadynamics as accurate binding free-energy method. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 6358-6363.	7.1	337
10	Isothermal-isobaric molecular dynamics using stochastic velocity rescaling. Journal of Chemical Physics, 2009, 130, 074101.	3.0	297
11	Flexible Docking in Solution Using Metadynamics. Journal of the American Chemical Society, 2005, 127, 2600-2607.	13.7	266
12	Well-Tempered Metadynamics Converges Asymptotically. Physical Review Letters, 2014, 112, 240602.	7.8	248
13	Freezing of a Lennard-Jones Fluid: From Nucleation to Spinodal Regime. Physical Review Letters, 2006, 97, 105701.	7.8	227
14	Variational Approach to Enhanced Sampling and Free Energy Calculations. Physical Review Letters, 2014, 113, 090601.	7.8	206
15	Uncovering Molecular Details of Urea Crystal Growth in the Presence of Additives. Journal of the American Chemical Society, 2012, 134, 17221-17233.	13.7	182
16	Molecular-dynamics simulations of urea nucleation from aqueous solution. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E6-14.	7.1	142
17	Silicon Liquid Structure and Crystal Nucleation from AbÂInitio Deep Metadynamics. Physical Review Letters, 2018, 121, 265701.	7.8	109
18	Deep learning the slow modes for rare events sampling. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	104

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19	Ab initio phase diagram and nucleation of gallium. Nature Communications, 2020, 11, 2654.	12.8	102
20	A variational conformational dynamics approach to the selection of collective variables in metadynamics. Journal of Chemical Physics, 2017, 147, 204109.	3.0	101
21	Collective Variables from Local Fluctuations. Journal of Physical Chemistry Letters, 2018, 9, 2776-2781.	4.6	101
22	The Unfolded Ensemble and Folding Mechanism of the C-Terminal GB1 Î²-Hairpin. Journal of the American Chemical Society, 2008, 130, 13938-13944.	13.7	97
23	Data-Driven Collective Variables for Enhanced Sampling. Journal of Physical Chemistry Letters, 2020, 11, 2998-3004.	4.6	97
24	Entropy based fingerprint for local crystalline order. Journal of Chemical Physics, 2017, 147, 114112.	3.0	92
25	Neural networks-based variationally enhanced sampling. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 17641-17647.	7.1	90
26	Controlling and Predicting Crystal Shapes: The Case of Urea. Angewandte Chemie - International Edition, 2013, 52, 13369-13372.	13.8	89
27	Metadynamics studies of crystal nucleation. IUCrJ, 2015, 2, 256-266.	2.2	84
28	Molecular dynamics simulations of liquid silica crystallization. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 5348-5352.	7.1	78
29	Enhancing Entropy and Enthalpy Fluctuations to Drive Crystallization in Atomistic Simulations. Physical Review Letters, 2017, 119, 015701.	7.8	74
30	A Minimum Free Energy Reaction Path for the E2 Reaction between Fluoro Ethane and a Fluoride Ion. Journal of the American Chemical Society, 2004, 126, 9492-9493.	13.7	73
31	Insight into the nucleation of urea crystals from the melt. Chemical Engineering Science, 2015, 121, 51-59.	3.8	70
32	Predicting polymorphism in molecular crystals using orientational entropy. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 10251-10256.	7.1	57
33	Chasing the Full Free Energy Landscape of Neuroreceptor/Ligand Unbinding by Metadynamics Simulations. Journal of Chemical Theory and Computation, 2019, 15, 3354-3361.	5.3	53
34	Enhanced, targeted sampling of high-dimensional free-energy landscapes using variationally enhanced sampling, with an application to chignolin. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 1150-1155.	7.1	47
35	Metadynamics with Discriminants: A Tool for Understanding Chemistry. Journal of Chemical Theory and Computation, 2018, 14, 5040-5044.	5.3	45
36	Thermoelectricity in Disordered Organic Semiconductors under the Premise of the Gaussian Disorder Model and Its Variants. Journal of Physical Chemistry Letters, 2014, 5, 3247-3253.	4.6	41

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37	Drift and Diffusion in Disordered Organic Semiconductors: The Role of Charge Density and Charge Energy Transport. Journal of Physical Chemistry C, 2013, 117, 3287-3293.	3.1	39
38	Improving collective variables: The case of crystallization. Journal of Chemical Physics, 2019, 150, 094509.	3.0	38
39	The role of water in host-guest interaction. Nature Communications, 2021, 12, 93.	12.8	37
40	Solvent-mediated morphology selection of the active pharmaceutical ingredient isoniazid: Experimental and simulation studies. Chemical Engineering Science, 2019, 204, 320-328.	3.8	35
41	Folding a small protein using harmonic linear discriminant analysis. Journal of Chemical Physics, 2018, 149, 194113.	3.0	34
42	Gaussian Mixture-Based Enhanced Sampling for Statics and Dynamics. Journal of Physical Chemistry Letters, 2020, 11, 5076-5080.	4.6	32
43	Molecular Dynamics Simulations of Crystal Nucleation from Solution at Constant Chemical Potential. Journal of Chemical Theory and Computation, 2019, 15, 6923-6930.	5.3	31
44	Integrating NMR and simulations reveals motions in the UUCG tetraloop. Nucleic Acids Research, 2020, 48, 5839-5848.	14.5	31
45	Exploration vs Convergence Speed in Adaptive-Bias Enhanced Sampling. Journal of Chemical Theory and Computation, 2022, 18, 3988-3996.	5.3	30
46	Microscopic description of acidâ€“base equilibrium. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 4054-4057.	7.1	28
47	Refining Collective Coordinates and Improving Free Energy Representation in Variational Enhanced Sampling. Journal of Chemical Theory and Computation, 2018, 14, 2889-2894.	5.3	25
48	Collective variables for the study of crystallisation. Molecular Physics, 2021, 119, .	1.7	25
49	Variational Flooding Study of a S_N2 Reaction. Journal of Physical Chemistry Letters, 2017, 8, 580-583.	4.6	23
50	The Onset of Dehydrogenation in Solid Ammonia Borane: An Ab Initio Metadynamics Study. Angewandte Chemie - International Edition, 2019, 58, 3976-3980.	13.8	23
51	Accurate Quantum Chemical Free Energies at Affordable Cost. Journal of Physical Chemistry Letters, 2019, 10, 3727-3731.	4.6	20
52	Blind Search for Complex Chemical Pathways Using Harmonic Linear Discriminant Analysis. Journal of Chemical Theory and Computation, 2019, 15, 4507-4515.	5.3	19
53	Naphthalene crystal shape prediction from molecular dynamics simulations. CrystEngComm, 2019, 21, 3280-3288.	2.6	19
54	A Cannibalistic Approach to Grand Canonical Crystal Growth. Journal of Chemical Theory and Computation, 2018, 14, 2678-2683.	5.3	18

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55	Searching for Entropically Stabilized Phases: The Case of Silver Iodide. Journal of Physical Chemistry C, 2018, 122, 1786-1790.	3.1	18
56	Making the Best of a Bad Situation: A Multiscale Approach to Free Energy Calculation. Journal of Chemical Theory and Computation, 2019, 15, 2187-2194.	5.3	18
57	Conformational Entropy as Collective Variable for Proteins. Journal of Physical Chemistry Letters, 2017, 8, 4752-4756.	4.6	16
58	Enhanced Sampling of Transition States. Journal of Chemical Theory and Computation, 2019, 15, 2454-2459.	5.3	16
59	From Enhanced Sampling to Reaction Profiles. Journal of Physical Chemistry Letters, 2021, 12, 8621-8626.	4.6	16
60	The Onset of Dehydrogenation in Solid Ammonia Borane: An Ab Initio Metadynamics Study. Angewandte Chemie, 2019, 131, 4016-4020.	2.0	14
61	Solubility Prediction of Organic Molecules with Molecular Dynamics Simulations. Crystal Growth and Design, 2021, 21, 5198-5205.	3.0	14
62	Identifying Slow Molecular Motions in Complex Chemical Reactions. Journal of Physical Chemistry Letters, 2017, 8, 4197-4200.	4.6	12
63	Discover, Sample, and Refine: Exploring Chemistry with Enhanced Sampling Techniques. Journal of Physical Chemistry Letters, 2022, 13, 1424-1430.	4.6	12
64	The Topology of Hopping in the Energy Domain of Systems with Rapidly Decaying Density of States. Journal of Physical Chemistry C, 2013, 117, 24740-24745.	3.1	10
65	Field dependent thermoelectric properties of organic semiconductorsâ€"A tool to determine the nature of charge transport in materials exhibiting thermally activated transport. Journal of Applied Physics, 2015, 117, 105502.	2.5	9
66	Rigorous analysis of image force barrier lowering in bounded geometries: application to semiconducting nanowires. Nanotechnology, 2014, 25, 145203.	2.6	6
67	Collective Variables for Free Energy Surface Tailoring: Understanding and Modifying Functionality in Systems Dominated by Rare Events. Journal of Physical Chemistry Letters, 2022, 13, 2830-2837.	4.6	5
68	A local fingerprint for hydrophobicity and hydrophilicity: From methane to peptides. Journal of Chemical Physics, 2019, 150, 204103.	3.0	4
69	Computing Rates and Understanding Unbinding Mechanisms in Hostâ€"Guest Systems. Journal of Chemical Theory and Computation, 2022, 18, 1314-1319.	5.3	4
70	A metadynamics perspective on the reduction mechanism of the Pt(IV) asplatin prodrug. Journal of Computational Chemistry, 2020, 41, 290-294.	3.3	3
71	Breviarium de Motu Simulato Ad Atomos Pertinenti. Israel Journal of Chemistry, 2022, 62, .	2.3	3
72	Solubility of Organic Salts in Solventâ€"Antisolvent Mixtures: A Combined Experimental and Molecular Dynamics Simulations Approach. Journal of Chemical Theory and Computation, 2022, 18, 4952-4959.	5.3	3