

Dan Mendels

List of Publications by Year in descending order

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papers

28,824
citations

94269

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82410

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73
docs citations

73
times ranked

26185
citing authors

#	ARTICLE	IF	CITATIONS
1	Breviarium de Motu Simulato Ad Atomos Pertinenti. Israel Journal of Chemistry, 2022, 62, .	1.0	3
2	Discover, Sample, and Refine: Exploring Chemistry with Enhanced Sampling Techniques. Journal of Physical Chemistry Letters, 2022, 13, 1424-1430.	2.1	12
3	Computing Rates and Understanding Unbinding Mechanisms in Host-Guest Systems. Journal of Chemical Theory and Computation, 2022, 18, 1314-1319.	2.3	4
4	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.	2.1	5
5	Exploration vs Convergence Speed in Adaptive-Bias Enhanced Sampling. Journal of Chemical Theory and Computation, 2022, 18, 3988-3996.	2.3	30
6	Solubility of Organic Salts in Solvent-Antisolvent Mixtures: A Combined Experimental and Molecular Dynamics Simulations Approach. Journal of Chemical Theory and Computation, 2022, 18, 4952-4959.	2.3	3
7	The role of water in host-guest interaction. Nature Communications, 2021, 12, 93.	5.8	37
8	Collective variables for the study of crystallisation. Molecular Physics, 2021, 119, .	0.8	25
9	Solubility Prediction of Organic Molecules with Molecular Dynamics Simulations. Crystal Growth and Design, 2021, 21, 5198-5205.	1.4	14
10	From Enhanced Sampling to Reaction Profiles. Journal of Physical Chemistry Letters, 2021, 12, 8621-8626.	2.1	16
11	Deep learning the slow modes for rare events sampling. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	104
12	A metadynamics perspective on the reduction mechanism of the Pt(IV) asplatin prodrug. Journal of Computational Chemistry, 2020, 41, 290-294.	1.5	3
13	Integrating NMR and simulations reveals motions in the UUCG tetraloop. Nucleic Acids Research, 2020, 48, 5839-5848.	6.5	31
14	Ab initio phase diagram and nucleation of gallium. Nature Communications, 2020, 11, 2654.	5.8	102
15	Gaussian Mixture-Based Enhanced Sampling for Statics and Dynamics. Journal of Physical Chemistry Letters, 2020, 11, 5076-5080.	2.1	32
16	Data-Driven Collective Variables for Enhanced Sampling. Journal of Physical Chemistry Letters, 2020, 11, 2998-3004.	2.1	97
17	Blind Search for Complex Chemical Pathways Using Harmonic Linear Discriminant Analysis. Journal of Chemical Theory and Computation, 2019, 15, 4507-4515.	2.3	19
18	Molecular Dynamics Simulations of Crystal Nucleation from Solution at Constant Chemical Potential. Journal of Chemical Theory and Computation, 2019, 15, 6923-6930.	2.3	31

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19	Neural networks-based variationally enhanced sampling. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 17641-17647.	3.3	90
20	The Onset of Dehydrogenation in Solid Ammonia Borane: An Ab Initio Metadynamics Study. Angewandte Chemie - International Edition, 2019, 58, 3976-3980.	7.2	23
21	Accurate Quantum Chemical Free Energies at Affordable Cost. Journal of Physical Chemistry Letters, 2019, 10, 3727-3731.	2.1	20
22	A local fingerprint for hydrophobicity and hydrophilicity: From methane to peptides. Journal of Chemical Physics, 2019, 150, 204103.	1.2	4
23	Naphthalene crystal shape prediction from molecular dynamics simulations. CrystEngComm, 2019, 21, 3280-3288.	1.3	19
24	Making the Best of a Bad Situation: A Multiscale Approach to Free Energy Calculation. Journal of Chemical Theory and Computation, 2019, 15, 2187-2194.	2.3	18
25	Chasing the Full Free Energy Landscape of Neuroreceptor/Ligand Unbinding by Metadynamics Simulations. Journal of Chemical Theory and Computation, 2019, 15, 3354-3361.	2.3	53
26	Improving collective variables: The case of crystallization. Journal of Chemical Physics, 2019, 150, 094509.	1.2	38
27	Enhanced Sampling of Transition States. Journal of Chemical Theory and Computation, 2019, 15, 2454-2459.	2.3	16
28	The Onset of Dehydrogenation in Solid Ammonia Borane: An Ab Initio Metadynamics Study. Angewandte Chemie, 2019, 131, 4016-4020.	1.6	14
29	Microscopic description of acid-base equilibrium. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 4054-4057.	3.3	28
30	Solvent-mediated morphology selection of the active pharmaceutical ingredient isoniazid: Experimental and simulation studies. Chemical Engineering Science, 2019, 204, 320-328.	1.9	35
31	A Cannibalistic Approach to Grand Canonical Crystal Growth. Journal of Chemical Theory and Computation, 2018, 14, 2678-2683.	2.3	18
32	Searching for Entropically Stabilized Phases: The Case of Silver Iodide. Journal of Physical Chemistry C, 2018, 122, 1786-1790.	1.5	18
33	Refining Collective Coordinates and Improving Free Energy Representation in Variational Enhanced Sampling. Journal of Chemical Theory and Computation, 2018, 14, 2889-2894.	2.3	25
34	Folding a small protein using harmonic linear discriminant analysis. Journal of Chemical Physics, 2018, 149, 194113.	1.2	34
35	Silicon Liquid Structure and Crystal Nucleation from <i>Ab Initio</i> Deep Metadynamics. Physical Review Letters, 2018, 121, 265701.	2.9	109
36	Metadynamics with Discriminants: A Tool for Understanding Chemistry. Journal of Chemical Theory and Computation, 2018, 14, 5040-5044.	2.3	45

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37	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.	3.3	57
38	Molecular dynamics simulations of liquid silica crystallization. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 5348-5352.	3.3	78
39	Collective Variables from Local Fluctuations. Journal of Physical Chemistry Letters, 2018, 9, 2776-2781.	2.1	101
40	Variational Flooding Study of a S_{N2} Reaction. Journal of Physical Chemistry Letters, 2017, 8, 580-583.	2.1	23
41	Entropy based fingerprint for local crystalline order. Journal of Chemical Physics, 2017, 147, 114112.	1.2	92
42	Identifying Slow Molecular Motions in Complex Chemical Reactions. Journal of Physical Chemistry Letters, 2017, 8, 4197-4200.	2.1	12
43	Conformational Entropy as Collective Variable for Proteins. Journal of Physical Chemistry Letters, 2017, 8, 4752-4756.	2.1	16
44	Enhancing Entropy and Enthalpy Fluctuations to Drive Crystallization in Atomistic Simulations. Physical Review Letters, 2017, 119, 015701.	2.9	74
45	A variational conformational dynamics approach to the selection of collective variables in metadynamics. Journal of Chemical Physics, 2017, 147, 204109.	1.2	101
46	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.	3.3	47
47	Enhancing Important Fluctuations: Rare Events and Metadynamics from a Conceptual Viewpoint. Annual Review of Physical Chemistry, 2016, 67, 159-184.	4.8	497
48	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.	3.3	142
49	Insight into the nucleation of urea crystals from the melt. Chemical Engineering Science, 2015, 121, 51-59.	1.9	70
50	Metadynamics studies of crystal nucleation. IUCr, 2015, 2, 256-266.	1.0	84
51	Field dependent thermoelectric properties of organic semiconductors—A tool to determine the nature of charge transport in materials exhibiting thermally activated transport. Journal of Applied Physics, 2015, 117, 105502.	1.1	9
52	A Time-Independent Free Energy Estimator for Metadynamics. Journal of Physical Chemistry B, 2015, 119, 736-742.	1.2	399
53	Rigorous analysis of image force barrier lowering in bounded geometries: application to semiconducting nanowires. Nanotechnology, 2014, 25, 145203.	1.3	6
54	Well-Tempered Metadynamics Converges Asymptotically. Physical Review Letters, 2014, 112, 240602.	2.9	248

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55	Variational Approach to Enhanced Sampling and Free Energy Calculations. <i>Physical Review Letters</i> , 2014, 113, 090601.	2.9	206
56	Thermoelectricity in Disordered Organic Semiconductors under the Premise of the Gaussian Disorder Model and Its Variants. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 3247-3253.	2.1	41
57	The Topology of Hopping in the Energy Domain of Systems with Rapidly Decaying Density of States. <i>Journal of Physical Chemistry C</i> , 2013, 117, 24740-24745.	1.5	10
58	Controlling and Predicting Crystal Shapes: The Case of Urea. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 13369-13372.	7.2	89
59	Funnel metadynamics as accurate binding free-energy method. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 6358-6363.	3.3	337
60	Drift and Diffusion in Disordered Organic Semiconductors: The Role of Charge Density and Charge Energy Transport. <i>Journal of Physical Chemistry C</i> , 2013, 117, 3287-3293.	1.5	39
61	Uncovering Molecular Details of Urea Crystal Growth in the Presence of Additives. <i>Journal of the American Chemical Society</i> , 2012, 134, 17221-17233.	6.6	182
62	Isothermal-isobaric molecular dynamics using stochastic velocity rescaling. <i>Journal of Chemical Physics</i> , 2009, 130, 074101.	1.2	297
63	Well-Tempered Metadynamics: A Smoothly Converging and Tunable Free-Energy Method. <i>Physical Review Letters</i> , 2008, 100, 020603.	2.9	2,201
64	The Unfolded Ensemble and Folding Mechanism of the C-Terminal GB1 $\hat{\text{I}}^2$ -Hairpin. <i>Journal of the American Chemical Society</i> , 2008, 130, 13938-13944.	6.6	97
65	From A to B in free energy space. <i>Journal of Chemical Physics</i> , 2007, 126, 054103.	1.2	476
66	Canonical sampling through velocity rescaling. <i>Journal of Chemical Physics</i> , 2007, 126, 014101.	1.2	11,867
67	Freezing of a Lennard-Jones Fluid: From Nucleation to Spinodal Regime. <i>Physical Review Letters</i> , 2006, 97, 105701.	2.9	227
68	Free-Energy Landscape for $\hat{\text{I}}^2$ Hairpin Folding from Combined Parallel Tempering and Metadynamics. <i>Journal of the American Chemical Society</i> , 2006, 128, 13435-13441.	6.6	458
69	Quickstep: Fast and accurate density functional calculations using a mixed Gaussian and plane waves approach. <i>Computer Physics Communications</i> , 2005, 167, 103-128.	3.0	4,200
70	Flexible Docking in Solution Using Metadynamics. <i>Journal of the American Chemical Society</i> , 2005, 127, 2600-2607.	6.6	266
71	A Minimum Free Energy Reaction Path for the E2 Reaction between Fluoro Ethane and a Fluoride Ion. <i>Journal of the American Chemical Society</i> , 2004, 126, 9492-9493.	6.6	73
72	Escaping free-energy minima. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002, 99, 12562-12566.	3.3	4,527