David J Wales

List of Publications by Year
in descending order

319 papers	22,774 citations	8732 75 h-index	10127 140 g-index
325 all docs	325 docs citations	325 times ranked	12964 citing authors

#	Article	IF	Citations
1	Global Optimization by Basin-Hopping and the Lowest Energy Structures of Lennard-Jones Clusters Containing up to 110 Atoms. Journal of Physical Chemistry A, 1997, 101, 5111-5116.	1.1	2,579
2	Theoretical studies of icosahedral C60 and some related species. Chemical Physics Letters, 1986, 128, 501-503.	1.2	1,789
3	Global Optimization of Clusters, Crystals, and Biomolecules. Science, 1999, 285, 1368-1372.	6.0	995
4	Archetypal energy landscapes. Nature, 1998, 394, 758-760.	13.7	528
5	Global minima of water clusters (H2O)n, nâ‰21, described by an empirical potential. Chemical Physics Letters, 1998, 286, 65-72.	1.2	405
6	The effect of the range of the potential on the structures of clusters. Journal of Chemical Physics, 1995, 103, 4234-4249.	1.2	380
7	Defect migration in crystalline silicon. Physical Review B, 1999, 59, 3969-3980.	1.1	371
8	Discrete path sampling. Molecular Physics, 2002, 100, 3285-3305.	0.8	359
9	A doubly nudged elastic band method for finding transition states. Journal of Chemical Physics, 2004, 120, 2082-2094.	1.2	356
10	Prediction of Sepsis in the Intensive Care Unit With Minimal Electronic Health Record Data: A Machine Learning Approach. JMIR Medical Informatics, 2016, 4, e28.	1.3	331
11	The double-funnel energy landscape of the 38-atom Lennard-Jones cluster. Journal of Chemical Physics, 1999, 110, 6896-6906.	1.2	279
12	Concerted hydrogen-bond breaking by quantum tunneling in the water hexamer prism. Science, 2016, 351, 1310-1313.	6.0	256
13	Evolution of the potential energy surface with size for Lennard-Jones clusters. Journal of Chemical Physics, 1999, 111, 8417-8428.	1.2	222
14	Structural consequences of the range of the interatomic potential A menagerie of clusters. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 4233-4243.	1.7	216
15	Thermodynamics of Global Optimization. Physical Review Letters, 1998, 80, 1357-1360.	2.9	208
16	Coexistence in small inert gas clusters. Molecular Physics, 1993, 78, 151-171.	0.8	198
17	A Microscopic Basis for the Global Appearance of Energy Landscapes. Science, 2001, 293, 2067-2070.	6.0	198
18	Virulence-Associated Substitution D222G in the Hemagglutinin of 2009 Pandemic Influenza A(H1N1) Virus Affects Receptor Binding. Journal of Virology, 2010, 84, 11802-11813.	1.5	197

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19	Some further applications of discrete path sampling to cluster isomerization. Molecular Physics, 2004, 102, 891-908.	0.8	190
20	Potential Energy and Free Energy Landscapes. Journal of Physical Chemistry B, 2006, 110, 20765-20776.	1.2	181
21	Thermodynamics and the global optimization of Lennard-Jones clusters. Journal of Chemical Physics, 1998, 109, 8143-8153.	1.2	178
22	From Topographies to Dynamics on Multidimensional Potential Energy Surfaces of Atomic Clusters. Science, 1996, 271, 963-966.	6.0	173
23	Saddle points and dynamics of Lennard-Jones clusters, solids, and supercooled liquids. Journal of Chemical Physics, 2002, 116, 3777-3788.	1.2	172
24	Energy landscapes: calculating pathways and rates. International Reviews in Physical Chemistry, 2006, 25, 237-282.	0.9	169
25	Theoretical study of water trimer. Journal of the American Chemical Society, 1993, 115, 11180-11190.	6.6	161
26	Thermodynamics and Kinetics of Aggregation for the GNNQQNY Peptide. Journal of the American Chemical Society, 2007, 129, 16005-16014.	6.6	161
27	Membrane Protein Structure, Function, and Dynamics: a Perspective from Experiments and Theory. Journal of Membrane Biology, 2015, 248, 611-640.	1.0	157
28	The energy landscape as a unifying theme in molecular science. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2005, 363, 357-377.	1.6	156
29	STATISTICAL THERMODYNAMICS: Taking a Walk on a Landscape. Science, 2001, 293, 612-613.	6.0	156
30	Transition states and rearrangement mechanisms from hybrid eigenvector-following and density functional theory.. Chemical Physics Letters, 2001, 341, 185-194.	1.2	155
31	Energy Landscapes: From Clusters to Biomolecules. Advances in Chemical Physics, 2007, , 1-111.	0.3	153
32	Finding pathways between distant local minima. Journal of Chemical Physics, 2005, 122, 234903.	1.2	152
33	Structure, Dynamics, and Thermodynamics of Clusters: Tales from Topographic Potential Surfaces. Science, 1996, 271, 925-929.	6.0	150
34	Calculation of thermodynamic properties of small Lennardâ€Jones clusters incorporating anharmonicity. Journal of Chemical Physics, 1995, 102, 9659-9672.	1.2	146
35	Free energy landscapes of model peptides and proteins. Journal of Chemical Physics, 2003, 118, 3891-3897.	1.2	143
36	Stationary points and dynamics in high-dimensional systems. Journal of Chemical Physics, 2003, 119, 12409-12416.	1.2	142

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37	The Structure and Stability of Atomic Liquids: From Clusters to Bulk. Science, 1996, 271, 484-487.	6.0	140
38	The effect of the range of the potential on the structure and stability of simple liquids: from clusters to bulk, from sodium to. Journal of Physics B: Atomic, Molecular and Optical Physics, 1996, 29, 4859-4894.	0.6	138
39	Transmembrane Structures for Alzheimerâ€™s AÎ²_{1â€“42} Oligomers. Journal of the American Chemical Society, 2010, 132, 13300-13312.	6.6	136
40	Folding of the GB1 hairpin peptide from discrete path sampling. Journal of Chemical Physics, 2004, 121, 1080-1090.	1.2	133
41	Energy landscapes: some new horizons. Current Opinion in Structural Biology, 2010, 20, 3-10.	2.6	133
42	How the range of pair interactions governs features of multidimensional potentials. Journal of Chemical Physics, 1990, 93, 8745-8756.	1.2	131
43	Structure and energetics of model metal clusters. Journal of Chemical Physics, 1992, 96, 8520-8534.	1.2	130
44	Theoretical study of the water pentamer. Journal of Chemical Physics, 1996, 105, 6957-6971.	1.2	127
45	Free energy barriers to melting in atomic clusters. Journal of Chemical Physics, 1994, 101, 1460-1476.	1.2	121
46	Structure and dynamics of spherical crystals characterized for the Thomson problem. Physical Review B, 2006, 74, .	1.1	118
47	Quantum partition functions from classical distributions: Application to rare-gas clusters. Journal of Chemical Physics, 2001, 114, 7312-7329.	1.2	117
48	Energy landscape of a model protein. Journal of Chemical Physics, 1999, 111, 6610-6616.	1.2	115
49	Structural relaxation in Morse clusters: Energy landscapes. Journal of Chemical Physics, 1999, 110, 328-334.	1.2	114
50	Free energy surfaces from an extended harmonic superposition approach and kinetics for alanine dipeptide. Chemical Physics Letters, 2008, 466, 105-115.	1.2	109
51	Energy landscapes of some model glass formers. Physical Review B, 2001, 64, .	1.1	104
52	Chaos in small clusters of inert gas atoms. Journal of Chemical Physics, 1992, 96, 1376-1390.	1.2	102
53	Rearrangements of model (H2O)8 and (H2O)20 clusters. Journal of Chemical Physics, 1993, 98, 7257-7268.	1.2	99
54	Prediction of early unplanned intensive care unit readmission in a UK tertiary care hospital: a cross-sectional machine learning approach. BMJ Open, 2017, 7, e017199.	0.8	95

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55	Folding Pathways and Rates for the Three-Stranded Î²-Sheet Peptide Beta3s using Discrete Path Sampling. Journal of Physical Chemistry B, 2008, 112, 8760-8769.	1.2	93
56	Exploring Energy Landscapes. Annual Review of Physical Chemistry, 2018, 69, 401-425.	4.8	93
57	On potential energy surfaces and relaxation to the global minimum. Journal of Chemical Physics, 1996, 105, 8428-8445.	1.2	92
58	Rearrangements of the water trimer. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 2505.	1.7	91
59	Global optimization and folding pathways of selected Î±-helical proteins. Journal of Chemical Physics, 2005, 123, 234901.	1.2	91
60	Locating stationary points for clusters in cartesian coordinates. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 1305.	1.7	90
61	Equilibrium thermodynamics from basin-sampling. Journal of Chemical Physics, 2006, 124, 044102.	1.2	89
62	Surveying a potential energy surface by eigenvector-following Applications to global optimisation and the structural transformations of clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1997, 40, 194-197.	1.0	86
63	Structural relaxation in atomic clusters: Master equation dynamics. Physical Review E, 1999, 60, 3701-3718.	0.8	86
64	Coexistence and phase separation in clusters: From the small to the notâ€soâ€small regime. Journal of Chemical Physics, 1995, 103, 3061-3070.	1.2	84
65	Theoretical study of the water tetramer. Journal of Chemical Physics, 1997, 106, 7193-7207.	1.2	84
66	Mapping Surface Hydrophobicity of Î±-Synuclein Oligomers at the Nanoscale. Nano Letters, 2018, 18, 7494-7501.	4.5	83
67	Finding saddle points for clusters. Journal of Chemical Physics, 1989, 91, 7002-7010.	1.2	82
68	Structure and torsional dynamics of the water octamer from THz laser spectroscopy near 215 Î¼m. Science, 2016, 352, 1194-1197.	6.0	82
69	Energy landscapes for diffusion: Analysis of cage-breaking processes. Journal of Chemical Physics, 2008, 129, 164507.	1.2	80
70	Instanton calculations of tunneling splittings for water dimer and trimer. Journal of Chemical Physics, 2011, 135, 124109.	1.2	80
71	Intrinsically Disordered Energy Landscapes. Scientific Reports, 2015, 5, 10386.	1.6	80
72	An order parameter approach to coexistence in atomic clusters. Journal of Chemical Physics, 1995, 102, 9673-9688.	1.2	79

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73	Calculating rate constants and committor probabilities for transition networks by graph transformation. Journal of Chemical Physics, 2009, 130, 204111.	1.2	79
74	Energy landscapes of model polyalanines. Journal of Chemical Physics, 2002, 117, 1363-1376.	1.2	78
75	Energy landscapes, global optimization and dynamics of the polyalanine Ac(ala)8NHMe. Journal of Chemical Physics, 2001, 114, 6443-6454.	1.2	77
76	Crystals of binary Lennard-Jones solids. Physical Review B, 2001, 64, .	1.1	77
77	The favored cluster structures of model glass formers. Journal of Chemical Physics, 2003, 118, 2792.	1.2	77
78	Exploring biomolecular energy landscapes. Chemical Communications, 2017, 53, 6974-6988.	2.2	77
79	Defect motifs for spherical topologies. Physical Review B, 2009, 79, .	1.1	76
80	Perspective: Insight into reaction coordinates and dynamics from the potential energy landscape. Journal of Chemical Physics, 2015, 142, 130901.	1.2	76
81	Basins of attraction for stationary points on a potential-energy surface. Journal of the Chemical Society, Faraday Transactions, 1992, 88, 653.	1.7	74
82	Temperature Controls Guest Uptake and Release from Zn₄L₄ Tetrahedra. Journal of the American Chemical Society, 2019, 141, 14534-14538.	6.6	74
83	The free energy landscape and dynamics of met-enkephalin. Journal of Chemical Physics, 2003, 119, 9947-9955.	1.2	71
84	Energy landscapes for machine learning. Physical Chemistry Chemical Physics, 2017, 19, 12585-12603.	1.3	71
85	Energy landscapes of model glasses. II. Results for constant pressure. Journal of Chemical Physics, 2003, 118, 4583-4593.	1.2	70
86	Theoretical study of rearrangements in water dimer and trimer. Molecular Physics, 2002, 100, 2793-2806.	0.8	67
87	Symmetry, near-symmetry and energetics. Chemical Physics Letters, 1998, 285, 330-336.	1.2	65
88	Decoding the energy landscape: extracting structure, dynamics and thermodynamics. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2012, 370, 2877-2899.	1.6	65
89	Symmetrisation schemes for global optimisation of atomic clusters. Physical Chemistry Chemical Physics, 2013, 15, 3965.	1.3	64
90	Energy Landscapes of Clusters Bound by Shortâ€Ranged Potentials. ChemPhysChem, 2010, 11, 2491-2494.	1.0	63

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91	Pinning Down the Water Hexamer. Science, 2012, 336, 814-815.	6.0	63
92	Energy Landscapes for Proteins: From Single Funnels to Multifunctional Systems. Advanced Theory and Simulations, 2019, 2, 1800175.	1.3	62
93	Emergent Complexity from Simple Anisotropic Building Blocks: Shells, Tubes, and Spirals. ACS Nano, 2010, 4, 219-228.	7.3	58
94	Surveying a complex potential energy landscape: Overcoming broken ergodicity using basin-sampling. Chemical Physics Letters, 2013, 584, 1-9.	1.2	57
95	The structure of (C60)N clusters. Chemical Physics Letters, 1996, 262, 167-174.	1.2	56
96	Characterization of anharmonicities on complex potential energy surfaces: Perturbation theory and simulation. Journal of Chemical Physics, 2001, 115, 9627-9636.	1.2	56
97	Observation time scale, free-energy landscapes, and molecular symmetry. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 617-622.	3.3	56
98	Decoupled Associative and Dissociative Processes in Strong yet Highly Dynamic Hostâ€“Guest Complexes. Journal of the American Chemical Society, 2017, 139, 12985-12993.	6.6	56
99	Local interpretation of chaotic dynamics in a many-body classical Hamiltonian system (Ar3). Journal of Physics B: Atomic, Molecular and Optical Physics, 1991, 24, L351-L357.	0.6	55
100	How many dimensions are required to approximate the potential energy landscape of a model protein?. Journal of Chemical Physics, 2005, 122, 084714.	1.2	53
101	Simulations of rigid bodies in an angle-axis framework. Physical Chemistry Chemical Physics, 2009, 11, 1970.	1.3	53
102	Energy landscapes of colloidal clusters: thermodynamics and rearrangement mechanisms. Nanoscale, 2012, 4, 1085-1100.	2.8	52
103	Investigation of Terahertz Vibrationâ€“Rotation Tunneling Spectra for the Water Octamer. Journal of Physical Chemistry A, 2013, 117, 6960-6966.	1.1	52
104	Relaxation dynamics of C60. Journal of Chemical Physics, 1998, 109, 6691-6700.	1.2	51
105	Ab initio study of rearrangements between C60 fullerenes. Chemical Physics Letters, 2003, 374, 125-131.	1.2	50
106	Coarse-Grained Simulations Complemented by Atomistic Molecular Dynamics Provide New Insights into Folding and Unfolding of Human Telomeric G-Quadruplexes. Journal of Chemical Theory and Computation, 2016, 12, 6077-6097.	2.3	50
107	Graph transformation method for calculating waiting times in Markov chains. Journal of Chemical Physics, 2006, 124, 234110.	1.2	49
108	Turning intractable counting into sampling: Computing the configurational entropy of three-dimensional jammed packings. Physical Review E, 2016, 93, 012906.	0.8	48

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109	Connectivity in the potential energy landscape for binary Lennard-Jones systems. Journal of Chemical Physics, 2009, 130, 194508.	1.2	47
110	Energy Landscapes, Folding Mechanisms, and Kinetics of RNA Tetraloop Hairpins. Journal of the American Chemical Society, 2014, 136, 18052-18061.	6.6	47
111	Dynamics and thermodynamics of supercooled liquids and glasses from a model energy landscape. Physical Review B, 2001, 63, .	1.1	45
112	Pathways for dissociative methane chemisorption onPt{110}â˜'(1Ã—2). Physical Review B, 2005, 71, .	1.1	45
113	Global minima of transition metal clusters described by Finnisâ€“Sinclair potentials: A comparison with semi-empirical molecular orbital theory. Philosophical Magazine, 2009, 89, 3311-3332.	0.7	44
114	Energy landscapes for shells assembled from pentagonal and hexagonal pyramids. Physical Chemistry Chemical Physics, 2009, 11, 2098.	1.3	44
115	Benchmarks for Characterization of Minima, Transition States, and Pathways in Atomic, Molecular, and Condensed Matter Systems. Journal of Chemical Theory and Computation, 2014, 10, 5476-5482.	2.3	43
116	Comparison of double-ended transition state search methods. Journal of Chemical Physics, 2007, 127, 134102.	1.2	42
117	Protein structure prediction using basin-hopping. Journal of Chemical Physics, 2008, 128, 225106.	1.2	42
118	The Energy Landscape, Folding Pathways and the Kinetics of a Knotted Protein. PLoS Computational Biology, 2010, 6, e1000835.	1.5	41
119	Designed to yield. Nature Materials, 2011, 10, 410-411.	13.3	41
120	The dynamics of structural transitions in sodium chloride clusters. Journal of Chemical Physics, 1999, 111, 11070-11079.	1.2	40
121	Kinetic analysis of discrete path sampling stationary point databases. Molecular Physics, 2006, 104, 1497-1507.	0.8	40
122	Refined kinetic transition networks for the GB1 hairpin peptide. Physical Chemistry Chemical Physics, 2009, 11, 3341.	1.3	40
123	Proline provides site-specific flexibility for in vivo collagen. Scientific Reports, 2018, 8, 13809.	1.6	40
124	Nested sampling for physical scientists. Nature Reviews Methods Primers, 2022, 2, .	11.8	40
125	Energy landscapes and properties of biomolecules. Physical Biology, 2005, 2, S86-S93.	0.8	39
126	Clusters of C60 molecules. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 1061.	1.7	37

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127	Comparison of kinetic Monte Carlo and molecular dynamics simulations of diffusion in a model glass former. Journal of Chemical Physics, 2004, 120, 8134-8143.	1.2	37
128	Rational design of helical architectures. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 20164-20167.	3.3	37
129	Mode-Specific Chemisorption of CH₄ on Pt{110}-(1 Ã— 2) Explored by First-Principles Molecular Dynamics. Journal of Physical Chemistry C, 2011, 115, 21832-21842.	1.5	37
130	Evolution of the Potential Energy Landscape with Static Pulling Force for Two Model Proteins. Journal of Physical Chemistry B, 2012, 116, 8394-8411.	1.2	37
131	Symmetrization of the AMBER and CHARMM force fields. Journal of Computational Chemistry, 2010, 31, 1402-1409.	1.5	36
132	A Local Rigid Body Framework for Global Optimization of Biomolecules. Journal of Chemical Theory and Computation, 2012, 8, 5159-5165.	2.3	36
133	Visualizing Basins of Attraction for Different Minimization Algorithms. Journal of Physical Chemistry B, 2013, 117, 12717-12723.	1.2	36
134	Structure, thermodynamics, and rearrangement mechanisms in gold clustersâ€"insights from the energy landscapes framework. Nanoscale, 2018, 10, 2004-2016.	2.8	36
135	What can calculations employing empirical potentials teach us about bare transition-metal clusters?. Journal of the Chemical Society Dalton Transactions, 1996, , 611.	1.1	35
136	Bifurcation tunneling dynamics in the water trimer. Journal of Chemical Physics, 2002, 117, 8823-8835.	1.2	35
137	Quasi-Continuous Interpolation Scheme for Pathways between Distant Configurations. Journal of Chemical Theory and Computation, 2012, 8, 5020-5034.	2.3	35
138	Designing a Bernal Spiral from Patchy Colloids. ACS Nano, 2013, 7, 1246-1256.	7.3	35
139	Quantum tunneling splittings from path-integral molecular dynamics. Journal of Chemical Physics, 2016, 144, 114108.	1.2	34
140	Decoding heat capacity features from the energy landscape. Physical Review E, 2017, 95, 030105.	0.8	34
141	Energy Landscape and Pathways for Transitions between Watsonâ€"Crick and Hoogsteen Base Pairing in DNA. Journal of Physical Chemistry Letters, 2018, 9, 229-241.	2.1	34
142	Tunneling splittings from path-integral molecular dynamics using a Langevin thermostat. Journal of Chemical Physics, 2018, 148, 234102.	1.2	34
143	Structural predictions for (C60)N clusters with an all-atom potential. Chemical Physics Letters, 1997, 269, 408-412.	1.2	33
144	Mode-specificity and transition state-specific energy redistribution in the chemisorption of CH4 on Ni{100}. Physical Chemistry Chemical Physics, 2012, 14, 15879.	1.3	33

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145	Structures and Energy Landscapes of Hydrated Sulfate Clusters. Journal of Chemical Theory and Computation, 2015, 11, 2377-2384.	2.3	33
146	Energy landscapes, structural topologies and rearrangement mechanisms in clusters of dipolar particles. Soft Matter, 2013, 9, 5407.	1.2	32
147	Communication: A new paradigm for structure prediction in multicomponent systems. Journal of Chemical Physics, 2013, 139, 221101.	1.2	32
148	Multifunctional energy landscape for a DNA G-quadruplex: An evolved molecular switch. Journal of Chemical Physics, 2017, 147, 152715.	1.2	32
149	Tunneling Splittings in Water Clusters from Path Integral Molecular Dynamics. Journal of Physical Chemistry Letters, 2019, 10, 7300-7304.	2.1	32
150	Potential energy surfaces and coordinate dependence. Journal of Chemical Physics, 2000, 113, 3926-3927.	1.2	31
151	Energy Landscape and Global Optimization for a Frustrated Model Protein. Journal of Physical Chemistry B, 2011, 115, 11525-11529.	1.2	30
152	Hydroxyproline Ring Pucker Causes Frustration of Helix Parameters in the Collagen Triple Helix. Scientific Reports, 2015, 5, 12556.	1.6	30
153	New results for phase transitions from catastrophe theory. Journal of Chemical Physics, 2004, 120, 11090-11099.	1.2	29
154	Dynamics of a molecular glass former: Energy landscapes for diffusion in ortho-terphenyl. Journal of Chemical Physics, 2016, 145, 024505.	1.2	29
155	A stress tensor eigenvector projection space for the (H2O)5 potential energy surface. Chemical Physics Letters, 2017, 667, 25-31.	1.2	29
156	Energy Landscapes for the Aggregation of Aî²_{17â€“42}. Journal of the American Chemical Society, 2018, 140, 4018-4027.	6.6	29
157	An ab initio study of tunneling splittings in the water dimer. Journal of Chemical Physics, 2004, 120, 5993-5999.	1.2	28
158	Pathways for dissociative ethane chemisorption on Pt{110} (1Ã—2) using density functional theory. Chemical Physics Letters, 2005, 413, 289-293.	1.2	28
159	Energetically favoured defects in dense packings of particles on spherical surfaces. Soft Matter, 2016, 12, 5708-5717.	1.2	28
160	Closed-shell structures and the building game. Chemical Physics Letters, 1987, 141, 478-484.	1.2	27
161	An ab initio study of tunneling splittings in the water trimer. Journal of Chemical Physics, 2005, 123, 044302.	1.2	27
162	Structure Prediction for Multicomponent Materials Using Biminima. Physical Review Letters, 2014, 113, 156102.	2.9	26

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163	Grand and Semigrand Canonical Basin-Hopping. Journal of Chemical Theory and Computation, 2016, 12, 902-909.	2.3	26
164	Evolved Minimal Frustration in Multifunctional Biomolecules. Journal of Physical Chemistry B, 2018, 122, 10989-10995.	1.2	26
165	Communication: Analysing kinetic transition networks for rare events. Journal of Chemical Physics, 2014, 141, 041104.	1.2	25
166	A conformational factorisation approach for estimating the binding free energies of macromolecules. Physical Chemistry Chemical Physics, 2014, 16, 2842-2853.	1.3	25
167	Design principles for Bernal spirals and helices with tunable pitch. Nanoscale, 2014, 6, 9448-9456.	2.8	25
168	Quasi-combinatorial energy landscapes for nanoalloy structure optimisation. Physical Chemistry Chemical Physics, 2015, 17, 28331-28338.	1.3	25
169	Transforming the Accuracy and Numerical Stability of ReaxFF Reactive Force Fields. Journal of Physical Chemistry Letters, 2019, 10, 7215-7223.	2.1	25
170	Super-Arrhenius Diffusion in an Undercooled Binary Lennard-Jones Liquid Results from a Quantifiable Correlation Effect. Physical Review Letters, 2006, 96, 057802.	2.9	24
171	Rovibrational transitions of the methaneâ€“water dimer from intermolecular quantum dynamical computations. Physical Chemistry Chemical Physics, 2016, 18, 22816-22826.	1.3	24
172	Archetypal energy landscapes: Dynamical diagnosis. Journal of Chemical Physics, 2005, 122, 024103.	1.2	23
173	Mapping Structural Changes in Electrode Materials: Application of the Hybrid Eigenvector-Following Density Functional Theory (DFT) Method to Layered Li_{0.5}MnO₂. Chemistry of Materials, 2015, 27, 5550-5561.	3.2	23
174	Coarse-graining the structure of polycyclic aromatic hydrocarbons clusters. Physical Chemistry Chemical Physics, 2016, 18, 13736-13740.	1.3	23
175	Improving Computational Predictions of Single-Stranded RNA Tetramers with Revised Î±/Î³ Torsional Parameters for the Amber Force Field. Journal of Physical Chemistry B, 2017, 121, 2989-2999.	1.2	23
176	Defining and quantifying frustration in the energy landscape: Applications to atomic and molecular clusters, biomolecules, jammed and glassy systems. Journal of Chemical Physics, 2017, 146, 124103.	1.2	23
177	Correlation effects and super-Arrhenius diffusion in binary Lennard-Jones mixtures. Physical Review B, 2006, 74, .	1.1	22
178	Analysis of cooperativity and localization for atomic rearrangements. Journal of Chemical Physics, 2004, 121, 6689-6697.	1.2	21
179	Exploring Energy Landscapes: Metrics, Pathways, and Normal-Mode Analysis for Rigid-Body Molecules. Journal of Chemical Theory and Computation, 2013, 9, 4026-4034.	2.3	21
180	Superposition Enhanced Nested Sampling. Physical Review X, 2014, 4, .	2.8	21

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181	Kinetic Transition Networks for the Thomson Problem and Smaleâ€™s Seventh Problem. Physical Review Letters, 2016, 117, 028301.	2.9	21
182	Energy landscapes for a machine learning application to series data. Journal of Chemical Physics, 2016, 144, 124119.	1.2	21
183	Probing helical transitions in a DNA duplex. Physical Chemistry Chemical Physics, 2017, 19, 878-892.	1.3	21
184	Defining, Calculating, and Converging Observables of a Kinetic Transition Network. Journal of Chemical Theory and Computation, 2020, 16, 2661-2679.	2.3	21
185	Magic numbers and growth sequences of small face-centered-cubic and decahedral clusters. Chemical Physics Letters, 1995, 247, 339-347.	1.2	20
186	Comment on â€œQuasisaddles as relevant points of the potential energy surface in the dynamics of supercooled liquidsâ€•[J. Chem. Phys. 116, 10297 (2002)]. Journal of Chemical Physics, 2003, 118, 5263-5264.	1.2	20
187	Bond-selective energy redistribution in the chemisorption of CH3D and CD3H on Pt{110}-(1Ã—2): A first-principles molecular dynamics study. Computational and Theoretical Chemistry, 2012, 990, 144-151.	1.1	20
188	Free energy basin-hopping. Chemical Physics Letters, 2015, 625, 1-4.	1.2	20
189	Computational Investigation of RNA C<u>U</u>G Repeats Responsible for Myotonic Dystrophy 1. Journal of Chemical Theory and Computation, 2015, 11, 4943-4958.	2.3	20
190	Optimal Alignment of Structures for Finite and Periodic Systems. Journal of Chemical Theory and Computation, 2017, 13, 4914-4931.	2.3	20
191	Energy Landscape for Fold-Switching in Regulatory Protein RfaH. Journal of Chemical Theory and Computation, 2019, 15, 731-742.	2.3	20
192	Affinity-Selected Bicyclic Peptide G-Quadruplex Ligands Mimic a Protein-like Binding Mechanism. Journal of the American Chemical Society, 2020, 142, 8367-8373.	6.6	20
193	Mechanisms for H₂ Reduction on the PdO{101} Surface and the Pd{100}-(âˆš5 Ã—) Tj ETQq1 1 0.784314 rgBT /Overloc	1.5	19
194	Energy landscapes and global thermodynamics for alanine peptides. Journal of Chemical Physics, 2013, 139, 121909.	1.2	19
195	Pathways for diffusion in the potential energy landscape of the network glass former SiO2. Journal of Chemical Physics, 2017, 147, 152726.	1.2	19
196	Energy landscapes of planar colloidal clusters. Nanoscale, 2014, 6, 10717-10726.	2.8	18
197	Energy Landscapes and Hybridization Pathways for DNA Hexamer Duplexes. Journal of Physical Chemistry Letters, 2019, 10, 6771-6779.	2.1	18
198	Energy Landscapes for Electronic Structure. Journal of Chemical Theory and Computation, 2021, 17, 151-169.	2.3	18

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