David J Wales

List of Publications by Citations

314 papers	19,530 citations	71 h-index	132 g-index
325 ext. papers	21,112 ext. citations	5.7 avg, IF	7.34 L-index

#	Paper	IF	Citations
314	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	2.8	2197
313	Theoretical studies of icosahedral C60 and some related species. *Chemical Physics Letters*, **1986**, 128, 501-503	2.5	1603
312	Global optimization of clusters, crystals, and biomolecules. *Science*, **1999**, 285, 1368-72	33.3	881
311	Archetypal energy landscapes. *Nature*, **1998**, 394, 758-760	50.4	469
310	Global minima of water clusters (H2O)n, n⩾1, described by an empirical potential. *Chemical Physics Letters*, **1998**, 286, 65-72	2.5	375
309	The effect of the range of the potential on the structures of clusters. *Journal of Chemical Physics*, **1995**, 103, 4234-4249	3.9	352
308	Defect migration in crystalline silicon. *Physical Review B*, **1999**, 59, 3969-3980	3.3	336
307	Discrete path sampling. *Molecular Physics*, **2002**, 100, 3285-3305	1.7	309
306	A doubly nudged elastic band method for finding transition states. *Journal of Chemical Physics*, **2004**, 120, 2082-94	3.9	295
305	The double-funnel energy landscape of the 38-atom Lennard-Jones cluster. *Journal of Chemical Physics*, **1999**, 110, 6896-6906	3.9	249
304	Energy Landscapes: Applications to Clusters, Biomolecules and Glasses **2004**,		231
303	Prediction of Sepsis in the Intensive Care Unit With Minimal Electronic Health Record Data: A Machine Learning Approach. *JMIR Medical Informatics*, **2016**, 4, e28	3.6	224
302	Evolution of the potential energy surface with size for Lennard-Jones clusters. *Journal of Chemical Physics*, **1999**, 111, 8417-8428	3.9	206
301	Structural consequences of the range of the interatomic potential A menagerie of clusters. *Journal of the Chemical Society, Faraday Transactions*, **1997**, 93, 4233-4243		198
300	Thermodynamics of Global Optimization. *Physical Review Letters*, **1998**, 80, 1357-1360	7.4	193
299	Coexistence in small inert gas clusters. *Molecular Physics*, **1993**, 78, 151-171	1.7	185
298	Concerted hydrogen-bond breaking by quantum tunneling in the water hexamer prism. *Science*, **2016**, 351, 1310-3	33.3	182

297	A microscopic basis for the global appearance of energy landscapes. *Science*, **2001**, 293, 2067-70	33.3	179
296	Virulence-associated substitution D222G in the hemagglutinin of 2009 pandemic influenza A(H1N1) virus affects receptor binding. *Journal of Virology*, **2010**, 84, 11802-13	6.6	171
295	Some further applications of discrete path sampling to cluster isomerization. *Molecular Physics*, **2004**, 102, 891-908	1.7	163
294	Thermodynamics and the global optimization of Lennard-Jones clusters. *Journal of Chemical Physics* , **1998**, 109, 8143-8153	3.9	163
293	Energy landscapes: calculating pathways and rates. *International Reviews in Physical Chemistry*, **2006**, 25, 237-282	7	161
292	Saddle points and dynamics of Lennard-Jones clusters, solids, and supercooled liquids. *Journal of Chemical Physics*, **2002**, 116, 3777-3788	3.9	157
291	From Topographies to Dynamics on Multidimensional Potential Energy Surfaces of Atomic Clusters. *Science*, **1996**, 271, 963-966	33.3	157
290	Potential energy and free energy landscapes. *Journal of Physical Chemistry B*, **2006**, 110, 20765-76	3.4	152
289	Theoretical study of water trimer. *Journal of the American Chemical Society*, **1993**, 115, 11180-11190	16.4	148
288	Statistical thermodynamics. Taking a walk on a landscape. *Science*, **2001**, 293, 612-3	33.3	143
287	Thermodynamics and kinetics of aggregation for the GNNQQNY peptide. *Journal of the American Chemical Society*, **2007**, 129, 16005-14	16.4	139
286	Calculation of thermodynamic properties of small Lennard-Jones clusters incorporating anharmonicity. *Journal of Chemical Physics*, **1995**, 102, 9659-9672	3.9	139
285	Free energy landscapes of model peptides and proteins. *Journal of Chemical Physics*, **2003**, 118, 3891-3897	3.9	136
284	Transition states and rearrangement mechanisms from hybrid eigenvector-following and density functional theory.. *Chemical Physics Letters*, **2001**, 341, 185-194	2.5	136
283	The energy landscape as a unifying theme in molecular science. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2005**, 363, 357-75; discussion 375-7	3	135
282	Structure, Dynamics, and Thermodynamics of Clusters: Tales from Topographic Potential Surfaces. *Science*, **1996**, 271, 925-929	33.3	131
281	Finding pathways between distant local minima. *Journal of Chemical Physics*, **2005**, 122, 234903	3.9	130
280	Folding of the GB1 hairpin peptide from discrete path sampling. *Journal of Chemical Physics*, **2004**, 121, 1080-90	3.9	130

279	Stationary points and dynamics in high-dimensional systems. *Journal of Chemical Physics*, **2003**, 119, 12409-12416	3.9	166
278	The Structure and Stability of Atomic Liquids: From Clusters to Bulk. *Science*, **1996**, 271, 484-487	33.3	126
277	Energy Landscapes: From Clusters to Biomolecules. *Advances in Chemical Physics*, **2007**, 1-111		124
276	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	1.3	120
275	How the range of pair interactions governs features of multidimensional potentials. *Journal of Chemical Physics*, **1990**, 93, 8745-8756	3.9	120
274	Free energy barriers to melting in atomic clusters. *Journal of Chemical Physics*, **1994**, 101, 1460-1476	3.9	119
273	Transmembrane structures for Alzheimer's A[1-42) oligomers. *Journal of the American Chemical Society*, **2010**, 132, 13300-12	16.4	116
272	Energy landscapes: some new horizons. *Current Opinion in Structural Biology*, **2010**, 20, 3-10	8.1	116
271	Quantum partition functions from classical distributions: Application to rare-gas clusters. *Journal of Chemical Physics*, **2001**, 114, 7312-7329	3.9	114
270	Theoretical study of the water pentamer. *Journal of Chemical Physics*, **1996**, 105, 6957-6971	3.9	114
269	Structure and energetics of model metal clusters. *Journal of Chemical Physics*, **1992**, 96, 8520-8534	3.9	113
268	Energy landscape of a model protein. *Journal of Chemical Physics*, **1999**, 111, 6610-6616	3.9	107
267	Structural relaxation in Morse clusters: Energy landscapes. *Journal of Chemical Physics*, **1999**, 110, 328-334	3.9	106
266	Membrane Protein Structure, Function, and Dynamics: a Perspective from Experiments and Theory. *Journal of Membrane Biology*, **2015**, 248, 611-40	2.3	101
265	Free energy surfaces from an extended harmonic superposition approach and kinetics for alanine dipeptide. *Chemical Physics Letters*, **2008**, 466, 105-115	2.5	100
264	Chaos in small clusters of inert gas atoms. *Journal of Chemical Physics*, **1992**, 96, 1376-1390	3.9	99
263	Structure and dynamics of spherical crystals characterized for the Thomson problem. *Physical Review B*, **2006**, 74,	3.3	97
262	Energy landscapes of some model glass formers. *Physical Review B*, **2001**, 64,	3.3	96

261	Rearrangements of model (H2O)8 and (H2O)20 clusters. *Journal of Chemical Physics*, **1993**, 98, 7257-7268	3.9	96
260	Global optimization and folding pathways of selected alpha-helical proteins. *Journal of Chemical Physics*, **2005**, 123, 234901	3.9	89
259	Folding pathways and rates for the three-stranded beta-sheet peptide Beta3s using discrete path sampling. *Journal of Physical Chemistry B*, **2008**, 112, 8760-9	3.4	86
258	Rearrangements of the water trimer. *Journal of the Chemical Society, Faraday Transactions*, **1996**, 92, 2505		84
257	Locating stationary points for clusters in cartesian coordinates. *Journal of the Chemical Society, Faraday Transactions*, **1993**, 89, 1305		83
256	Equilibrium thermodynamics from basin-sampling. *Journal of Chemical Physics*, **2006**, 124, 044102	3.9	82
255	Coexistence and phase separation in clusters: From the small to the not-so-small regime. *Journal of Chemical Physics*, **1995**, 103, 3061-3070	3.9	81
254	On potential energy surfaces and relaxation to the global minimum. *Journal of Chemical Physics*, **1996**, 105, 8428-8445	3.9	79
253	Theoretical study of the water tetramer. *Journal of Chemical Physics*, **1997**, 106, 7193-7207	3.9	78
252	Surveying a potential energy surface by eigenvector-following. *Zeitschrift F□ Physik D-Atoms Molecules and Clusters*, **1997**, 40, 194-197		78
251	Energy landscapes of model polyalanines. *Journal of Chemical Physics*, **2002**, 117, 1363-1376	3.9	78
250	Energy landscapes, global optimization and dynamics of the polyalanine Ac(ala)8NHMe. *Journal of Chemical Physics*, **2001**, 114, 6443-6454	3.9	75
249	Structural relaxation in atomic clusters: master equation dynamics. *Physical Review E*, **1999**, 60, 3701-18	2.4	74
248	An order parameter approach to coexistence in atomic clusters. *Journal of Chemical Physics*, **1995**, 102, 9673-9688	3.9	74
247	The favored cluster structures of model glass formers. *Journal of Chemical Physics*, **2003**, 118, 2792	3.9	72
246	Finding saddle points for clusters. *Journal of Chemical Physics*, **1989**, 91, 7002-7010	3.9	72
245	Energy landscapes for diffusion: analysis of cage-breaking processes. *Journal of Chemical Physics*, **2008**, 129, 164507	3.9	71
244	The free energy landscape and dynamics of met-enkephalin. *Journal of Chemical Physics*, **2003**, 119, 9947-9955	3.9	71

243	Calculating rate constants and committor probabilities for transition networks by graph transformation. *Journal of Chemical Physics*, **2009**, 130, 204111	3.9	69
242	Crystals of binary Lennard-Jones solids. *Physical Review B*, **2001**, 64,	3.3	69
241	Basins of attraction for stationary points on a potential-energy surface. *Journal of the Chemical Society, Faraday Transactions*, **1992**, 88, 653		68
240	Perspective: Insight into reaction coordinates and dynamics from the potential energy landscape. *Journal of Chemical Physics*, **2015**, 142, 130901	3.9	66
239	Energy landscapes of model glasses. II. Results for constant pressure. *Journal of Chemical Physics*, **2003**, 118, 4583-4593	3.9	66
238	Instanton calculations of tunneling splittings for water dimer and trimer. *Journal of Chemical Physics*, **2011**, 135, 124109	3.9	65
237	Exploring Energy Landscapes. *Annual Review of Physical Chemistry*, **2018**, 69, 401-425	15.7	62
236	Theoretical study of rearrangements in water dimer and trimer. *Molecular Physics*, **2002**, 100, 2793-2806	1.7	62
235	Defect motifs for spherical topologies. *Physical Review B*, **2009**, 79,	3.3	59
234	Structure and torsional dynamics of the water octamer from THz laser spectroscopy near 215 ℏ. *Science*, **2016**, 352, 1194-7	33.3	58
233	Decoding the energy landscape: extracting structure, dynamics and thermodynamics. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2012**, 370, 2877-99	3	58
232	Energy landscapes of clusters bound by short-ranged potentials. *ChemPhysChem*, **2010**, 11, 2491-4	3.2	58
231	Energy landscapes for machine learning. *Physical Chemistry Chemical Physics*, **2017**, 19, 12585-12603	3.6	57
230	Chemistry. Pinning down the water hexamer. *Science*, **2012**, 336, 814-5	33.3	57
229	Characterization of anharmonicities on complex potential energy surfaces: Perturbation theory and simulation. *Journal of Chemical Physics*, **2001**, 115, 9627-9636	3.9	56
228	Intrinsically disordered energy landscapes. *Scientific Reports*, **2015**, 5, 10386	4.9	54
227	Symmetry, near-symmetry and energetics. *Chemical Physics Letters*, **1998**, 285, 330-336	2.5	54
226	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	1.3	53

225	Symmetrisation schemes for global optimisation of atomic clusters. *Physical Chemistry Chemical Physics*, **2013**, 15, 3965-76	3.6	51
224	Surveying a complex potential energy landscape: Overcoming broken ergodicity using basin-sampling. *Chemical Physics Letters*, **2013**, 584, 1-9	2.5	51
223	The structure of (C60)N clusters. *Chemical Physics Letters*, **1996**, 262, 167-174	2.5	51
222	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	3	50
221	Energy landscapes of colloidal clusters: thermodynamics and rearrangement mechanisms. *Nanoscale*, **2012**, 4, 1085-100	7.7	50
220	How many dimensions are required to approximate the potential energy landscape of a model protein?. *Journal of Chemical Physics*, **2005**, 122, 84714	3.9	49
219	Exploring biomolecular energy landscapes. *Chemical Communications*, **2017**, 53, 6974-6988	5.8	48
218	Emergent complexity from simple anisotropic building blocks: shells, tubes, and spirals. *ACS Nano*, **2010**, 4, 219-28	16.7	48
217	Simulations of rigid bodies in an angle-axis framework. *Physical Chemistry Chemical Physics*, **2009**, 11, 1970-6	3.6	48
216	Relaxation dynamics of C60. *Journal of Chemical Physics*, **1998**, 109, 6691-6700	3.9	48
215	Turning intractable counting into sampling: Computing the configurational entropy of three-dimensional jammed packings. *Physical Review E*, **2016**, 93, 012906	2.4	45
214	Observation time scale, free-energy landscapes, and molecular symmetry. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 617-22	11.5	44
213	Investigation of terahertz vibration-rotation tunneling spectra for the water octamer. *Journal of Physical Chemistry A*, **2013**, 117, 6960-6	2.8	44
212	Connectivity in the potential energy landscape for binary Lennard-Jones systems. *Journal of Chemical Physics*, **2009**, 130, 194508	3.9	44
211	Graph transformation method for calculating waiting times in Markov chains. *Journal of Chemical Physics*, **2006**, 124, 234110	3.9	44
210	Ab initio study of rearrangements between C60 fullerenes. *Chemical Physics Letters*, **2003**, 374, 125-131	2.5	44
209	Decoupled Associative and Dissociative Processes in Strong yet Highly Dynamic Host-Guest Complexes. *Journal of the American Chemical Society*, **2017**, 139, 12985-12993	16.4	43
208	Pathways for dissociative methane chemisorption on Pt{110}{1[illegible]2). *Physical Review B*, **2005**, 71,	3.3	42

207	Mapping Surface Hydrophobicity of α-Synuclein Oligomers at the Nanoscale. *Nano Letters*, **2018**, 18, 7494-7501	11.5	42
206	Dynamics and thermodynamics of supercooled liquids and glasses from a model energy landscape. *Physical Review B*, **2001**, 63,	3.3	41
205	Global minima of transition metal clusters described by Finnis-Sinclair potentials: A comparison with semi-empirical molecular orbital theory. *Philosophical Magazine*, **2009**, 89, 3311-3332	1.6	39
204	The dynamics of structural transitions in sodium chloride clusters. *Journal of Chemical Physics*, **1999**, 111, 11070-11079	3.9	39
203	Benchmarks for Characterization of Minima, Transition States, and Pathways in Atomic, Molecular, and Condensed Matter Systems. *Journal of Chemical Theory and Computation*, **2014**, 10, 5476-82	6.4	38
202	Comparison of double-ended transition state search methods. *Journal of Chemical Physics*, **2007**, 127, 134102	3.9	38
201	Energy landscapes, folding mechanisms, and kinetics of RNA tetraloop hairpins. *Journal of the American Chemical Society*, **2014**, 136, 18052-61	16.4	37
200	The energy landscape, folding pathways and the kinetics of a knotted protein. *PLoS Computational Biology*, **2010**, 6, e1000835	5	37
199	Protein structure prediction using basin-hopping. *Journal of Chemical Physics*, **2008**, 128, 225106	3.9	37
198	Rational design of helical architectures. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 20164-20167	11.5	36
197	Refined kinetic transition networks for the GB1 hairpin peptide. *Physical Chemistry Chemical Physics* , **2009**, 11, 3341-54	3.6	36
196	Energy landscapes and properties of biomolecules. *Physical Biology*, **2005**, 2, S86-93	3	36
195	Clusters of C60 molecules. *Journal of the Chemical Society, Faraday Transactions*, **1994**, 90, 1061		36
194	Energy Landscapes for Proteins: From Single Funnels to Multifunctional Systems. *Advanced Theory and Simulations*, **2019**, 2, 1800175	3.5	35
193	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	6.4	35
192	Designing a Bernal spiral from patchy colloids. *ACS Nano*, **2013**, 7, 1246-56	16.7	35
191	Energy landscapes for shells assembled from pentagonal and hexagonal pyramids. *Physical Chemistry Chemical Physics*, **2009**, 11, 2098-104	3.6	35
190	Comparison of kinetic Monte Carlo and molecular dynamics simulations of diffusion in a model glass former. *Journal of Chemical Physics*, **2004**, 120, 8134-43	3.9	35

189	Visualizing basins of attraction for different minimization algorithms. *Journal of Physical Chemistry B*, **2013**, 117, 12717-23	3.4	34
188	Kinetic analysis of discrete path sampling stationary point databases. *Molecular Physics*, **2006**, 104, 1497-1507	1.7	34
187	Mode-Specific Chemisorption of CH4 on Pt{110}-(1 □2) Explored by First-Principles Molecular Dynamics. *Journal of Physical Chemistry C*, **2011**, 115, 21832-21842	3.8	33
186	What can calculations employing empirical potentials teach us about bare transition-metal clusters?. *Journal of the Chemical Society Dalton Transactions*, **1996**, 611		33
185	A Local Rigid Body Framework for Global Optimization of Biomolecules. *Journal of Chemical Theory and Computation*, **2012**, 8, 5159-65	6.4	32
184	Bifurcation tunneling dynamics in the water trimer. *Journal of Chemical Physics*, **2002**, 117, 8823-8835	3.9	32
183	Structural predictions for (C60)N clusters with an all-atom potential. *Chemical Physics Letters*, **1997**, 269, 408-412	2.5	31
182	Potential energy surfaces and coordinate dependence. *Journal of Chemical Physics*, **2000**, 113, 3926-3927	3.9	30
181	Temperature Controls Guest Uptake and Release from ZnL Tetrahedra. *Journal of the American Chemical Society*, **2019**, 141, 14534-14538	16.4	29
180	Mode-specificity and transition state-specific energy redistribution in the chemisorption of CH4 on Ni{100}. *Physical Chemistry Chemical Physics*, **2012**, 14, 15879-87	3.6	29
179	Evolution of the potential energy landscape with static pulling force for two model proteins. *Journal of Physical Chemistry B*, **2012**, 116, 8394-411	3.4	29
178	Energy landscape and global optimization for a frustrated model protein. *Journal of Physical Chemistry B*, **2011**, 115, 11525-9	3.4	29
177	Energy landscapes, structural topologies and rearrangement mechanisms in clusters of dipolar particles. *Soft Matter*, **2013**, 9, 5407	3.6	28
176	Communication: a new paradigm for structure prediction in multicomponent systems. *Journal of Chemical Physics*, **2013**, 139, 221101	3.9	28
175	Pathways for dissociative ethane chemisorption on Pt{110} (1□2) using density functional theory. *Chemical Physics Letters*, **2005**, 413, 289-293	2.5	28
174	Structures and Energy Landscapes of Hydrated Sulfate Clusters. *Journal of Chemical Theory and Computation*, **2015**, 11, 2377-84	6.4	27
173	Energy Landscape and Pathways for Transitions between Watson-Crick and Hoogsteen Base Pairing in DNA. *Journal of Physical Chemistry Letters*, **2018**, 9, 229-241	6.4	27
172	Quasi-Continuous Interpolation Scheme for Pathways between Distant Configurations. *Journal of Chemical Theory and Computation*, **2012**, 8, 5020-34	6.4	27

171	New results for phase transitions from catastrophe theory. *Journal of Chemical Physics*, **2004**, 120, 11090-9	3.9	27
170	Symmetrization of the AMBER and CHARMM force fields. *Journal of Computational Chemistry*, **2010**, 31, 1402-9	3.5	26
169	Hydroxyproline Ring Pucker Causes Frustration of Helix Parameters in the Collagen Triple Helix. *Scientific Reports*, **2015**, 5, 12556	4.9	25
168	An ab initio study of tunneling splittings in the water trimer. *Journal of Chemical Physics*, **2005**, 123, 044303	3.9	25
167	Closed-shell structures and the building game. *Chemical Physics Letters*, **1987**, 141, 478-484	2.5	25
166	Structure, thermodynamics, and rearrangement mechanisms in gold clusters-insights from the energy landscapes framework. *Nanoscale*, **2018**, 10, 2004-2016	7.7	25
165	An ab initio study of tunneling splittings in the water dimer. *Journal of Chemical Physics*, **2004**, 120, 5993-9	3.9	24
164	Quantum tunneling splittings from path-integral molecular dynamics. *Journal of Chemical Physics*, **2016**, 144, 114108	3.9	24
163	Proline provides site-specific flexibility for in vivo collagen. *Scientific Reports*, **2018**, 8, 13809	4.9	24
162	Design principles for Bernal spirals and helices with tunable pitch. *Nanoscale*, **2014**, 6, 9448-56	7.7	23
161	Dynamics of a molecular glass former: Energy landscapes for diffusion in ortho-terphenyl. *Journal of Chemical Physics*, **2016**, 145, 024505	3.9	23
160	Energy Landscapes for the Aggregation of A *Journal of the American Chemical Society*, **2018**, 140, 4018-4027	14.4	22
159	Energetically favoured defects in dense packings of particles on spherical surfaces. *Soft Matter*, **2016**, 12, 5708-17	3.6	22
158	Multifunctional energy landscape for a DNA G-quadruplex: An evolved molecular switch. *Journal of Chemical Physics*, **2017**, 147, 152715	3.9	22
157	Archetypal energy landscapes: dynamical diagnosis. *Journal of Chemical Physics*, **2005**, 122, 024103	3.9	22
156	Decoding heat capacity features from the energy landscape. *Physical Review E*, **2017**, 95, 030105	2.4	21
155	Grand and Semigrand Canonical Basin-Hopping. *Journal of Chemical Theory and Computation*, **2016**, 12, 902-9	6.4	21
154	Super-Arrhenius diffusion in an undercooled binary Lennard-Jones liquid results from a quantifiable correlation effect. *Physical Review Letters*, **2006**, 96, 057802	7.4	21

153	Quasi-combinatorial energy landscapes for nanoalloy structure optimisation. *Physical Chemistry Chemical Physics*, **2015**, 17, 28331-8	3.6	20
152	Rovibrational transitions of the methane-water dimer from intermolecular quantum dynamical computations. *Physical Chemistry Chemical Physics*, **2016**, 18, 22816-26	3.6	20
151	Structure prediction for multicomponent materials using biminima. *Physical Review Letters*, **2014**, 113, 156102	7.4	20
150	Analysis of cooperativity and localization for atomic rearrangements. *Journal of Chemical Physics*, **2004**, 121, 6689-97	3.9	20
149	Energy landscapes for a machine learning application to series data. *Journal of Chemical Physics*, **2016**, 144, 124119	3.9	19
148	A stress tensor eigenvector projection space for the (H2O)5 potential energy surface. *Chemical Physics Letters*, **2017**, 667, 25-31	2.5	19
147	Communication: Analysing kinetic transition networks for rare events. *Journal of Chemical Physics*, **2014**, 141, 041104	3.9	19
146	Energy landscapes and global thermodynamics for alanine peptides. *Journal of Chemical Physics*, **2013**, 139, 121909	3.9	19
145	Mechanisms for H2 Reduction on the PdO{101} Surface and the Pd{100}-(□ □)R27°-O Surface Oxide. *Journal of Physical Chemistry C*, **2009**, 113, 16757-16765	3.8	19
144	Correlation effects and super-Arrhenius diffusion in binary Lennard-Jones mixtures. *Physical Review B*, **2006**, 74,	3.3	19
143	Probing helical transitions in a DNA duplex. *Physical Chemistry Chemical Physics*, **2016**, 19, 878-892	3.6	18
142	Free energy basin-hopping. *Chemical Physics Letters*, **2015**, 625, 1-4	2.5	18
141	Energy landscapes of planar colloidal clusters. *Nanoscale*, **2014**, 6, 10717-26	7.7	18
140	Superposition Enhanced Nested Sampling. *Physical Review X*, **2014**, 4,	9.1	18
139	Bond-selective energy redistribution in the chemisorption of CH3D and CD3H on Pt{110}-(1×2): A first-principles molecular dynamics study. *Computational and Theoretical Chemistry*, **2012**, 990, 144-151	2	18
138	Coarse-graining the structure of polycyclic aromatic hydrocarbons clusters. *Physical Chemistry Chemical Physics*, **2016**, 18, 13736-40	3.6	18
137	Improving Computational Predictions of Single-Stranded RNA Tetramers with Revised α/γ Torsional Parameters for the Amber Force Field. *Journal of Physical Chemistry B*, **2017**, 121, 2989-2999	3.4	17
136	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	3.9	17

135	Exploring Energy Landscapes: Metrics, Pathways, and Normal-Mode Analysis for Rigid-Body Molecules. *Journal of Chemical Theory and Computation*, **2013**, 9, 4026-34	6.4	17
134	Comment on "Quasisaddles as relevant points of the potential energy surface in the dynamics of supercooled liquids" [J. Chem. Phys. 116, 10297 (2002)]. *Journal of Chemical Physics*, **2003**, 118, 5263-5264	3.9	17
133	Computational investigation of RNA CUG repeats responsible for myotonic dystrophy 1. *Journal of Chemical Theory and Computation*, **2015**, 11, 4943-58	6.4	16
132	A conformational factorisation approach for estimating the binding free energies of macromolecules. *Physical Chemistry Chemical Physics*, **2014**, 16, 2842-53	3.6	16
131	Optimal Alignment of Structures for Finite and Periodic Systems. *Journal of Chemical Theory and Computation*, **2017**, 13, 4914-4931	6.4	16
130	Communication: Certifying the potential energy landscape. *Journal of Chemical Physics*, **2013**, 138, 171101	3.9	16
129	Coupled linear and rotary motion in supramolecular helix handedness inversion. *Soft Matter*, **2011**, 7, 2325	3.6	16
128	Tunneling splittings from path-integral molecular dynamics using a Langevin thermostat. *Journal of Chemical Physics*, **2018**, 148, 234102	3.9	16
127	Kinetic Transition Networks for the Thomson Problem and Smale's Seventh Problem. *Physical Review Letters*, **2016**, 117, 028301	7.4	15
126	GPU-Accelerated Exploration of Biomolecular Energy Landscapes. *Journal of Chemical Theory and Computation*, **2016**, 12, 6182-6191	6.4	15
125	Tunneling Splittings in Water Clusters from Path Integral Molecular Dynamics. *Journal of Physical Chemistry Letters*, **2019**, 10, 7300-7304	6.4	15
124	Exploring energy landscapes: from molecular to mesoscopic systems. *Physical Chemistry Chemical Physics*, **2014**, 16, 5014-25	3.6	15
123	Rearrangements of Water Dimer and Hexamer. *Springer Series in Cluster Physics*, **1999**, 86-110		15
122	Dynamics and thermodynamics of the coronene octamer described by coarse-grained potentials. *Physical Chemistry Chemical Physics*, **2017**, 19, 1884-1895	3.6	14
121	Energy landscapes for a machine-learning prediction of patient discharge. *Physical Review E*, **2016**, 93, 063310	2.4	14
120	Transforming the Accuracy and Numerical Stability of ReaxFF Reactive Force Fields. *Journal of Physical Chemistry Letters*, **2019**, 10, 7215-7223	6.4	14
119	A left-handed building block self-assembles into right- and left-handed helices. *RSC Advances*, **2013**, 3, 12905	3.7	14
118	Supercooled Lennard-Jones liquids and glasses: a kinetic Monte Carlo approach. *Journal of Non-Crystalline Solids*, **2004**, 336, 218-222	3.9	14

117	Diagnosing broken ergodicity using an energy fluctuation metric. *Journal of Chemical Physics*, **2005**, 123, 134504	3.9	14
116	Magic numbers and growth sequences of small face-centered-cubic and decahedral clusters. *Chemical Physics Letters*, **1995**, 247, 339-347	2.5	14
115	Reaction path zero-point energy from diffusion Monte Carlo calculations. *Journal of Chemical Physics*, **1995**, 102, 1592-1596	3.9	14
114	When do gradient optimisations converge to saddle points?. *Chemical Physics Letters*, **1992**, 190, 447-452	2.5	14
113	Pathways for diffusion in the potential energy landscape of the network glass former SiO. *Journal of Chemical Physics*, **2017**, 147, 152726	3.9	13
112	Mapping Structural Changes in Electrode Materials: Application of the Hybrid Eigenvector-Following Density Functional Theory (DFT) Method to Layered Li0.5MnO2. *Chemistry of Materials*, **2015**, 27, 5550-5561	9.6	13
111	Defining, Calculating, and Converging Observables of a Kinetic Transition Network. *Journal of Chemical Theory and Computation*, **2020**, 16, 2661-2679	6.4	13
110	From sticky-hard-sphere to Lennard-Jones-type clusters. *Physical Review E*, **2018**, 97, 043309	2.4	13
109	Chemistry, geometry, and defects in two dimensions. *ACS Nano*, **2014**, 8, 1081-5	16.7	13
108	Communication: Newton homotopies for sampling stationary points of potential energy landscapes. *Journal of Chemical Physics*, **2014**, 141, 121104	3.9	13
107	Interpolation schemes for peptide rearrangements. *Journal of Chemical Physics*, **2010**, 132, 054101	3.9	13
106	Self-assembly of colloidal magnetic particles: energy landscapes and structural transitions. *Physical Chemistry Chemical Physics*, **2016**, 18, 26579-26585	3.6	13
105	Impurity effects on solid-solid transitions in atomic clusters. *Nanoscale*, **2016**, 8, 18326-18340	7.7	13
104	Evolved Minimal Frustration in Multifunctional Biomolecules. *Journal of Physical Chemistry B*, **2018**, 122, 10989-10995	3.4	13
103	Transforming the Energy Landscape of a Coiled-Coil Peptide via Point Mutations. *Journal of Chemical Theory and Computation*, **2017**, 13, 1468-1477	6.4	12
102	What Makes Telomeres Unique?. *Journal of Physical Chemistry B*, **2017**, 121, 2207-2219	3.4	12
101	Identifying mechanistically distinct pathways in kinetic transition networks. *Journal of Chemical Physics*, **2019**, 151, 124101	3.9	12
100	Structural analysis of high-dimensional basins of attraction. *Physical Review E*, **2016**, 94, 031301	2.4	12

99	Rate constants, timescales, and free energy barriers. *Journal of Non-Equilibrium Thermodynamics*, **2016**, 41,	3.8	11
98	Structure and energetics of model symmetric and asymmetric decahedra. *The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties*, **1992**, 65, 1079-1096		11
97	Preventing Structural Rearrangements on Battery Cycling: A First-Principles Investigation of the Effect of Dopants on the Migration Barriers in Layered Li0.5MnO2. *Journal of Physical Chemistry C*, **2016**, 120, 19521-19530	3.8	11
96	Exploiting the potential energy landscape to sample free energy. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2015**, 5, 273-289	7.9	10
95	Properties of kinetic transition networks for atomic clusters and glassy solids. *Physical Chemistry Chemical Physics*, **2017**, 19, 25498-25508	3.6	10
94	A survey of the potential energy surface for the (benzene)13 cluster. *Physical Chemistry Chemical Physics*, **2011**, 13, 21362-6	3.6	10
93	Rearrangements and tunneling in water clusters. *Advances in Molecular Vibrations and Collision Dynamics*, **1998**, 365-396		10
92	Energy Landscapes for Electronic Structure. *Journal of Chemical Theory and Computation*, **2021**, 17, 151-169	6.4	10
91	The potential energy landscape for crystallisation of a Lennard-Jones fluid. *Journal of Statistical Mechanics: Theory and Experiment*, **2016**, 2016, 074001	1.9	10
90	Loss surface of XOR artificial neural networks. *Physical Review E*, **2018**, 97, 052307	2.4	10
89	Exploring the potential energy landscape of the Thomson problem via Newton homotopies. *Journal of Chemical Physics*, **2015**, 142, 194113	3.9	9
88	Rare events and first passage time statistics from the energy landscape. *Journal of Chemical Physics* , **2020**, 153, 134115	3.9	9
87	Conformational Energy Landscape of the Ritonavir Molecule. *Journal of Physical Chemistry B*, **2016**, 120, 4331-40	3.4	9
86	Energy Landscape for Fold-Switching in Regulatory Protein RfaH. *Journal of Chemical Theory and Computation*, **2019**, 15, 731-742	6.4	9
85	Path Integral Energy Landscapes for Water Clusters. *Journal of Chemical Theory and Computation*, **2019**, 15, 33-42	6.4	9
84	Effects of random pinning on the potential energy landscape of a supercooled liquid. *Journal of Chemical Physics*, **2018**, 149, 114503	3.9	9
83	Mutational Basin-Hopping: Combined Structure and Sequence Optimization for Biomolecules. *Journal of Physical Chemistry Letters*, **2018**, 9, 6169-6173	6.4	9
82	Markov state modeling and dynamical coarse-graining via discrete relaxation path sampling. *Journal of Chemical Physics*, **2015**, 143, 044119	3.9	8

81	Affinity-Selected Bicyclic Peptide G-Quadruplex Ligands Mimic a Protein-like Binding Mechanism. *Journal of the American Chemical Society*, **2020**, 142, 8367-8373	16.4	8
80	Superposition-Enhanced Estimation of Optimal Temperature Spacings for Parallel Tempering Simulations. *Journal of Chemical Theory and Computation*, **2014**, 10, 5599-5605	6.4	8
79	Structure and dynamics of model Ag and Pt clusters. *Zeitschrift F Physik D-Atoms Molecules and Clusters*, **1993**, 26, 258-260		8
78	Energy landscapes and persistent minima. *Journal of Chemical Physics*, **2016**, 144, 054109	3.9	8
77	QTAIM and stress tensor interpretation of the (H O) potential energy surface. *Journal of Computational Chemistry*, **2016**, 37, 2712-2721	3.5	8
76	Structural transitions in the RNA 7SK 5' hairpin and their effect on HEXIM binding. *Nucleic Acids Research*, **2020**, 48, 373-389	20.1	8
75	Atomic clusters with addressable complexity. *Journal of Chemical Physics*, **2017**, 146, 054306	3.9	7
74	Structure and Thermodynamics of Metal Clusters on Atomically Smooth Substrates. *Journal of Physical Chemistry Letters*, **2017**, 8, 5402-5407	6.4	7
73	Dynamics of an adenine-adenine RNA conformational switch from discrete path sampling. *Journal of Chemical Physics*, **2019**, 150, 125101	3.9	7
72	Terahertz VRT spectroscopy of the water hexamer-d12 prism: Dramatic enhancement of bifurcation tunneling upon librational excitation. *Journal of Chemical Physics*, **2018**, 148, 094301	3.9	7
71	Energy Landscapes and Hybridization Pathways for DNA Hexamer Duplexes. *Journal of Physical Chemistry Letters*, **2019**, 10, 6771-6779	6.4	7
70	An inversion-relaxation approach for sampling stationary points of spin model Hamiltonians. *Journal of Chemical Physics*, **2014**, 140, 194104	3.9	7
69	THE ENERGY LANDSCAPE AS A COMPUTATIONAL TOOL **2008**, 321-330		7
68	Efficient and exact sampling of transition path ensembles on Markovian networks. *Journal of Chemical Physics*, **2020**, 153, 024121	3.9	7
67	Intrinsically Disordered Landscapes for Human CD4 Receptor Peptide. *Journal of Physical Chemistry B*, **2018**, 122, 11906-11921	3.4	7
66	Energy Landscape of the Designed Protein Top7. *Journal of Physical Chemistry B*, **2018**, 122, 12282-12291	3.4	7
65	Machine learning prediction for classification of outcomes in local minimisation. *Chemical Physics Letters*, **2017**, 667, 158-164	2.5	6
64	Nested Basin-Sampling. *Journal of Chemical Theory and Computation*, **2019**, 15, 6865-6881	6.4	6

63	Go-Kit: A Tool To Enable Energy Landscape Exploration of Proteins. *Journal of Chemical Information and Modeling*, **2019**, 59, 1703-1708	6.1	6
62	Communication: optimal parameters for basin-hopping global optimization based on Tsallis statistics. *Journal of Chemical Physics*, **2014**, 141, 071101	3.9	6
61	Geometry optimization for peptides and proteins: comparison of Cartesian and internal coordinates. *Journal of Chemical Physics*, **2007**, 127, 234105	3.9	6
60	A well-behaved theoretical framework for ReaxFF reactive force fields. *Journal of Chemical Physics*, **2020**, 153, 021102	3.9	6
59	Design of a Kagome lattice from soft anisotropic particles. *Soft Matter*, **2015**, 11, 6663-8	3.6	5
58	Designing hierarchical molecular complexity: icosahedra of addressable icosahedra. *Molecular Physics*, **2018**, 116, 2954-2964	1.7	5
57	Structure, Thermodynamics, and Folding Pathways for a Tryptophan Zipper as a Function of Local Rigidification. *Journal of Chemical Theory and Computation*, **2016**, 12, 6109-6117	6.4	5
56	Predicting Pathways between Distant Configurations for Biomolecules. *Journal of Chemical Theory and Computation*, **2018**, 14, 4271-4278	6.4	5
55	The Contribution of Backbone Electrostatic Repulsion to DNA Mechanical Properties is Length-Scale-Dependent. *Journal of Physical Chemistry Letters*, **2019**, 10, 4829-4835	6.4	5
54	Proton transfer pathways, energy landscape, and kinetics in creatine-water systems. *Journal of Physical Chemistry B*, **2014**, 118, 1969-75	3.4	5
53	Certification and the potential energy landscape. *Journal of Chemical Physics*, **2014**, 140, 224114	3.9	5
52	Energy Landscapes and Structure Prediction Using Basin-Hopping **2010**, 29-54		5
51	Analysis of the Ub to Ub-CR Transition in Ubiquitin. *Biochemistry*, **2018**, 57, 6180-6186	3.2	5
50	Counterion-Trapped-Molecules: From High Polarity and Enriched IR Spectra to Induced Isomerization. *ChemPhysChem*, **2020**, 21, 348-355	3.2	4
49	Kinetics of Molecular Diffusion and Self-Assembly: Glycine on Cu{110}. *Journal of Physical Chemistry C*, **2018**, 122, 782-797	3.8	4
48	Chaotic dynamics near steep transition states. *Molecular Physics*, **2012**, 110, 1839-1848	1.7	4
47	Nearly reducible finite Markov chains: Theory and algorithms. *Journal of Chemical Physics*, **2021**, 155, 140901	3.9	4
46	Archetypal landscapes for deep neural networks. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 21857-21864	11.5	4

45	Energy Landscapes of Mini-Dumbbell DNA Octanucleotides. *Journal of Chemical Theory and Computation*, **2018**, 14, 3870-3876	6.4	4
44	Analysis of the Contrasting Pathogenicities Induced by the D222G Mutation in 1918 and 2009 Pandemic Influenza A Viruses. *Journal of Chemical Theory and Computation*, **2015**, 11, 2307-14	6.4	3
43	Energy Landscapes of Deoxyxylo- and Xylo-Nucleic Acid Octamers. *Journal of Physical Chemistry B*, **2020**, 124, 4062-4068	3.4	3
42	Computational Studies of the Mechanical Stability for Single-Strand Break DNA. *Journal of Physical Chemistry B*, **2018**, 122, 8166-8173	3.4	3
41	Terahertz VRT Spectroscopy of the Water Hexamer-h12 Cage: Dramatic Libration-Induced Enhancement of Hydrogen Bond Tunneling Dynamics. *Journal of Physical Chemistry A*, **2018**, 122, 7421-7426	2.8	3
40	Machine learning landscapes and predictions for patient outcomes. *Royal Society Open Science*, **2017**, 4, 170175	3.3	3
39	Energy landscapes of a hairpin peptide including NMR chemical shift restraints. *Physical Chemistry Chemical Physics*, **2015**, 17, 20250-8	3.6	3
38	Beryllium cluster cages endohedrally doped by hydrogen: H2@Ben (8 ≤ n ≤ 14). *International Journal of Quantum Chemistry*, **2012**, 112, 3068-3075	2.1	3
37	Optimal dimensionality reduction of Markov chains using graph transformation. *Journal of Chemical Physics*, **2020**, 153, 244108	3.9	3
36	A multifunnel energy landscape encodes the competing α-helix and β-hairpin conformations for a designed peptide. *Physical Chemistry Chemical Physics*, **2020**, 22, 1359-1370	3.6	3
35	Flip rearrangement in the water pentamer: Analysis of electronic structure. *International Journal of Quantum Chemistry*, **2020**, 120, e26124	2.1	3
34	Multifunnel Energy Landscapes for Phosphorylated Translation Repressor 4E-BP2 and Its Mutants. *Journal of Chemical Theory and Computation*, **2020**, 16, 800-810	6.4	3
33	Energy Landscape for the Membrane Fusion Pathway in Influenza A Hemagglutinin From Discrete Path Sampling. *Frontiers in Chemistry*, **2020**, 8, 575195	5	3
32	Protein energy landscape exploration with structure-based models. *Current Opinion in Structural Biology*, **2020**, 64, 145-151	8.1	3
31	Numerical analysis of first-passage processes in finite Markov chains exhibiting metastability. *Physical Review E*, **2021**, 104, 015301	2.4	3
30	Potential energy landscapes of tetragonal pyramid molecules. *Chemical Physics Letters*, **2016**, 664, 5-9	2.5	3
29	Exotic bilayer crystals in a strong magnetic field. *Physical Review B*, **2018**, 97,	3.3	3
28	Exploiting sparsity in free energy basin-hopping. *Chemical Physics Letters*, **2017**, 685, 288-293	2.5	2

27	Exploring Energy Landscapes with Monte Carlo Methods. *AIP Conference Proceedings*, **2003**,	0	2
26	Crystal Structure Prediction for Benzene Using Basin-Hopping Global Optimization. *Journal of Physical Chemistry A*, **2021**, 125, 3776-3784	2.8	2
25	Surface Chirality Influences Molecular Rotation upon Desorption. *Physical Review Letters*, **2021**, 126, 166101	7.4	2
24	Systematic Evaluation of ReaxFF Reactive Force Fields for Biochemical Applications. *Journal of Chemical Theory and Computation*, **2021**, 17, 497-514	6.4	2
23	Energy landscapes and dynamics of glycine on Cu(110). *Physical Chemistry Chemical Physics*, **2017**, 19, 16600-16605	3.6	1
22	Equilibrium molecular thermodynamics from Kirkwood sampling. *Journal of Physical Chemistry B*, **2015**, 119, 6155-69	3.4	1
21	Perspective: new insights from loss function landscapes of neural networks. *Machine Learning: Science and Technology*, **2020**, 1, 023002	5.1	1
20	Dynamical properties of two- and three-dimensional colloidal clusters of six particles. *Physical Chemistry Chemical Physics*, **2016**, 18, 12725-32	3.6	1
19	Energy Landscapes, Self-Assembly and Viruses. *Journal of Theoretical Medicine*, **2005**, 6, 107-110		1
18	Improving double-ended transition state searches for soft-matter systems. *Journal of Chemical Physics*, **2020**, 153, 034104	3.9	1
17	Fragility and correlated dynamics in supercooled liquids. *Journal of Chemical Physics*, **2020**, 153, 124501	3.9	1
16	Graph transformation and shortest paths algorithms for finite Markov chains. *Physical Review E*, **2021**, 103, 063306	2.4	1
15	Morphological analysis of chiral rod clusters from a coarse-grained single-site chiral potential. *Soft Matter*, **2019**, 15, 8147-8155	3.6	1
14	Computational Investigation of RNA A-Bulges Related to the Microtubule-Associated Protein Tau Causing Frontotemporal Dementia and Parkinsonism. *Journal of Physical Chemistry B*, **2019**, 123, 57-65	3.4	1
13	The energy landscapes of bidisperse particle assemblies on a sphere. *Soft Matter*, **2021**, 17, 9019-9027	3.6	1
12	Development of ReaxFF Reactive Force Field for Aqueous Iron-Sulfur Clusters with Applications to Stability and Reactivity in Water. *Journal of Chemical Information and Modeling*, **2021**, 61, 1204-1214	6.1	1
11	Rotational Dynamics of Desorption: Methane and Ethane at Stepped and Kinked Platinum Surfaces. *Journal of Physical Chemistry C*, **2021**, 125, 27938-27948	3.8	1
10	The Energy Landscape Perspective: Encoding Structure and Function for Biomolecules.. *Frontiers in Molecular Biosciences*, **2022**, 9, 820792	5.6	0

9	Trapping of hydrogen atoms inside small beryllium clusters and their ions. *Chemical Physics Letters*, **2016**, 659, 282-288	2.5	0
8	Minimal Design Principles for Icosahedral Virus Capsids. *ACS Nano*, **2021**, 15, 14873-14884	16.7	0
7	On the capacity and superposition of minima in neural network loss function landscapes. *Machine Learning: Science and Technology*, **2022**, 3, 025004	5.1	0
6	How to make a porphyrin flip: dynamics of asymmetric porphyrin oligomers. *Physical Chemistry Chemical Physics*, **2015**, 17, 27094-102	3.6	
5	Response to "Comment on 'Exploring the potential energy landscape of the Thomson problem via Newton homotopies"' [J. Chem. Phys. 143, 247101 (2015)]. *Journal of Chemical Physics*, **2015**, 143, 247102	3.9	
4	Characterising the area under the curve loss function landscape. *Machine Learning: Science and Technology*, **2022**, 3, 015019	5.1	
3	Elucidating the solution structure of the K-means cost function using energy landscape theory.. *Journal of Chemical Physics*, **2022**, 156, 054109	3.9	
2	Side-Chain Polarity Modulates the Intrinsic Conformational Landscape of Model Dipeptides. *Journal of Physical Chemistry B*, **2021**, 125, 5809-5822	3.4	
1	The energy landscape perspective: cutting a Gordian knot. *Frontiers of Nanoscience*, **2022**, 1-18	0.7	