David J Wales

List of Publications by Year in Descending Order

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	The Energy Landscape Perspective: Encoding Structure and Function for Biomolecules.. *Frontiers in Molecular Biosciences*, **2022**, 9, 820792	5.6	0
313	Characterising the area under the curve loss function landscape. *Machine Learning: Science and Technology*, **2022**, 3, 015019	5.1	
312	Elucidating the solution structure of the K-means cost function using energy landscape theory.. *Journal of Chemical Physics*, **2022**, 156, 054109	3.9	
311	On the capacity and superposition of minima in neural network loss function landscapes. *Machine Learning: Science and Technology*, **2022**, 3, 025004	5.1	0
310	The energy landscape perspective: cutting a Gordian knot. *Frontiers of Nanoscience*, **2022**, 1-18	0.7	
309	Nearly reducible finite Markov chains: Theory and algorithms. *Journal of Chemical Physics*, **2021**, 155, 140901	3.9	4
308	Energy Landscapes for Electronic Structure. *Journal of Chemical Theory and Computation*, **2021**, 17, 151-169	5.4	10
307	Crystal Structure Prediction for Benzene Using Basin-Hopping Global Optimization. *Journal of Physical Chemistry A*, **2021**, 125, 3776-3784	2.8	2
306	Surface Chirality Influences Molecular Rotation upon Desorption. *Physical Review Letters*, **2021**, 126, 166101	7.4	2
305	Side-Chain Polarity Modulates the Intrinsic Conformational Landscape of Model Dipeptides. *Journal of Physical Chemistry B*, **2021**, 125, 5809-5822	3.4	
304	Graph transformation and shortest paths algorithms for finite Markov chains. *Physical Review E*, **2021**, 103, 063306	2.4	1
303	Numerical analysis of first-passage processes in finite Markov chains exhibiting metastability. *Physical Review E*, **2021**, 104, 015301	2.4	3
302	Systematic Evaluation of ReaxFF Reactive Force Fields for Biochemical Applications. *Journal of Chemical Theory and Computation*, **2021**, 17, 497-514	6.4	2
301	The energy landscapes of bidisperse particle assemblies on a sphere. *Soft Matter*, **2021**, 17, 9019-9027	3.6	1
300	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
299	Minimal Design Principles for Icosahedral Virus Capsids. *ACS Nano*, **2021**, 15, 14873-14884	16.7	0
298	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

297	Perspective: new insights from loss function landscapes of neural networks. *Machine Learning: Science and Technology*, **2020**, 1, 023002	5.1	1
296	Defining, Calculating, and Converging Observables of a Kinetic Transition Network. *Journal of Chemical Theory and Computation*, **2020**, 16, 2661-2679	6.4	13
295	Counterion-Trapped-Molecules: From High Polarity and Enriched IR Spectra to Induced Isomerization. *ChemPhysChem*, **2020**, 21, 348-355	3.2	4
294	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
293	Energy Landscapes of Deoxyxylo- and Xylo-Nucleic Acid Octamers. *Journal of Physical Chemistry B*, **2020**, 124, 4062-4068	3.4	3
292	Optimal dimensionality reduction of Markov chains using graph transformation. *Journal of Chemical Physics*, **2020**, 153, 244108	3.9	3
291	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
290	Flip rearrangement in the water pentamer: Analysis of electronic structure. *International Journal of Quantum Chemistry*, **2020**, 120, e26124	2.1	3
289	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
288	Energy Landscape for the Membrane Fusion Pathway in Influenza A Hemagglutinin From Discrete Path Sampling. *Frontiers in Chemistry*, **2020**, 8, 575195	5	3
287	Rare events and first passage time statistics from the energy landscape. *Journal of Chemical Physics* , **2020**, 153, 134115	3.9	9
286	A well-behaved theoretical framework for ReaxFF reactive force fields. *Journal of Chemical Physics*, **2020**, 153, 021102	3.9	6
285	Efficient and exact sampling of transition path ensembles on Markovian networks. *Journal of Chemical Physics*, **2020**, 153, 024121	3.9	7
284	Improving double-ended transition state searches for soft-matter systems. *Journal of Chemical Physics*, **2020**, 153, 034104	3.9	1
283	Protein energy landscape exploration with structure-based models. *Current Opinion in Structural Biology*, **2020**, 64, 145-151	8.1	3
282	Fragility and correlated dynamics in supercooled liquids. *Journal of Chemical Physics*, **2020**, 153, 124501	3.9	1
281	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
280	Structural transitions in the RNA 7SK 5' hairpin and their effect on HEXIM binding. *Nucleic Acids Research*, **2020**, 48, 373-389	20.1	8

279	Temperature Controls Guest Uptake and Release from ZnL Tetrahedra. *Journal of the American Chemical Society*, **2019**, 141, 14534-14538	16.4	29
278	Nested Basin-Sampling. *Journal of Chemical Theory and Computation*, **2019**, 15, 6865-6881	6.4	6
277	Energy Landscapes for Proteins: From Single Funnels to Multifunctional Systems. *Advanced Theory and Simulations*, **2019**, 2, 1800175	3.5	35
276	Go-Kit: A Tool To Enable Energy Landscape Exploration of Proteins. *Journal of Chemical Information and Modeling*, **2019**, 59, 1703-1708	6.1	6
275	Dynamics of an adenine-adenine RNA conformational switch from discrete path sampling. *Journal of Chemical Physics*, **2019**, 150, 125101	3.9	7
274	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
273	Identifying mechanistically distinct pathways in kinetic transition networks. *Journal of Chemical Physics*, **2019**, 151, 124101	3.9	12
272	Energy Landscapes and Hybridization Pathways for DNA Hexamer Duplexes. *Journal of Physical Chemistry Letters*, **2019**, 10, 6771-6779	6.4	7
271	Tunneling Splittings in Water Clusters from Path Integral Molecular Dynamics. *Journal of Physical Chemistry Letters*, **2019**, 10, 7300-7304	6.4	15
270	Transforming the Accuracy and Numerical Stability of ReaxFF Reactive Force Fields. *Journal of Physical Chemistry Letters*, **2019**, 10, 7215-7223	6.4	14
269	Morphological analysis of chiral rod clusters from a coarse-grained single-site chiral potential. *Soft Matter*, **2019**, 15, 8147-8155	3.6	1
268	Energy Landscape for Fold-Switching in Regulatory Protein RfaH. *Journal of Chemical Theory and Computation*, **2019**, 15, 731-742	6.4	9
267	Path Integral Energy Landscapes for Water Clusters. *Journal of Chemical Theory and Computation*, **2019**, 15, 33-42	6.4	9
266	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
265	Energy Landscapes for the Aggregation of A *Journal of the American Chemical Society*, **2018**, 140, 4018-4027	16.4	22
264	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
263	Exploring Energy Landscapes. *Annual Review of Physical Chemistry*, **2018**, 69, 401-425	15.7	62
262	From sticky-hard-sphere to Lennard-Jones-type clusters. *Physical Review E*, **2018**, 97, 043309	2.4	13

261	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
260	Kinetics of Molecular Diffusion and Self-Assembly: Glycine on Cu{110}. *Journal of Physical Chemistry C*, **2018**, 122, 782-797	3.8	4
259	Designing hierarchical molecular complexity: icosahedra of addressable icosahedra. *Molecular Physics*, **2018**, 116, 2954-2964	1.7	5
258	Computational Studies of the Mechanical Stability for Single-Strand Break DNA. *Journal of Physical Chemistry B*, **2018**, 122, 8166-8173	3.4	3
257	Predicting Pathways between Distant Configurations for Biomolecules. *Journal of Chemical Theory and Computation*, **2018**, 14, 4271-4278	6.4	5
256	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
255	Structure, thermodynamics, and rearrangement mechanisms in gold clusters-insights from the energy landscapes framework. *Nanoscale*, **2018**, 10, 2004-2016	7.7	25
254	Intrinsically Disordered Landscapes for Human CD4 Receptor Peptide. *Journal of Physical Chemistry B*, **2018**, 122, 11906-11921	3.4	7
253	Energy Landscape of the Designed Protein Top7. *Journal of Physical Chemistry B*, **2018**, 122, 12282-12291	3.4	7
252	Analysis of the Ub to Ub-CR Transition in Ubiquitin. *Biochemistry*, **2018**, 57, 6180-6186	3.2	5
251	Effects of random pinning on the potential energy landscape of a supercooled liquid. *Journal of Chemical Physics*, **2018**, 149, 114503	3.9	9
250	Mutational Basin-Hopping: Combined Structure and Sequence Optimization for Biomolecules. *Journal of Physical Chemistry Letters*, **2018**, 9, 6169-6173	6.4	9
249	Mapping Surface Hydrophobicity of □Synuclein Oligomers at the Nanoscale. *Nano Letters*, **2018**, 18, 7494-7501	11.5	42
248	Proline provides site-specific flexibility for in vivo collagen. *Scientific Reports*, **2018**, 8, 13809	4.9	24
247	Loss surface of XOR artificial neural networks. *Physical Review E*, **2018**, 97, 052307	2.4	10
246	Energy Landscapes of Mini-Dumbbell DNA Octanucleotides. *Journal of Chemical Theory and Computation*, **2018**, 14, 3870-3876	6.4	4
245	Evolved Minimal Frustration in Multifunctional Biomolecules. *Journal of Physical Chemistry B*, **2018**, 122, 10989-10995	3.4	13
244	Tunneling splittings from path-integral molecular dynamics using a Langevin thermostat. *Journal of Chemical Physics*, **2018**, 148, 234102	3.9	16

243	Exotic bilayer crystals in a strong magnetic field. *Physical Review B*, **2018**, 97,	3.3	3
242	Machine learning prediction for classification of outcomes in local minimisation. *Chemical Physics Letters*, **2017**, 667, 158-164	2.5	6
241	Atomic clusters with addressable complexity. *Journal of Chemical Physics*, **2017**, 146, 054306	3.9	7
240	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
239	What Makes Telomeres Unique?. *Journal of Physical Chemistry B*, **2017**, 121, 2207-2219	3.4	12
238	Exploring biomolecular energy landscapes. *Chemical Communications*, **2017**, 53, 6974-6988	5.8	48
237	Energy landscapes and dynamics of glycine on Cu(110). *Physical Chemistry Chemical Physics*, **2017**, 19, 16600-16605	3.6	1
236	Energy landscapes for machine learning. *Physical Chemistry Chemical Physics*, **2017**, 19, 12585-12603	3.6	57
235	Decoding heat capacity features from the energy landscape. *Physical Review E*, **2017**, 95, 030105	2.4	21
234	Improving Computational Predictions of Single-Stranded RNA Tetramers with Revised $\alpha\gamma$ Torsional Parameters for the Amber Force Field. *Journal of Physical Chemistry B*, **2017**, 121, 2989-2999	3.4	17
233	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
232	Dynamics and thermodynamics of the coronene octamer described by coarse-grained potentials. *Physical Chemistry Chemical Physics*, **2017**, 19, 1884-1895	3.6	14
231	Pathways for diffusion in the potential energy landscape of the network glass former SiO. *Journal of Chemical Physics*, **2017**, 147, 152726	3.9	13
230	Structure and Thermodynamics of Metal Clusters on Atomically Smooth Substrates. *Journal of Physical Chemistry Letters*, **2017**, 8, 5402-5407	6.4	7
229	Optimal Alignment of Structures for Finite and Periodic Systems. *Journal of Chemical Theory and Computation*, **2017**, 13, 4914-4931	6.4	16
228	Properties of kinetic transition networks for atomic clusters and glassy solids. *Physical Chemistry Chemical Physics*, **2017**, 19, 25498-25508	3.6	10
227	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
226	Exploiting sparsity in free energy basin-hopping. *Chemical Physics Letters*, **2017**, 685, 288-293	2.5	2

225	Machine learning landscapes and predictions for patient outcomes. *Royal Society Open Science*, **2017**, 4, 170175	3.3	3
224	Multifunctional energy landscape for a DNA G-quadruplex: An evolved molecular switch. *Journal of Chemical Physics*, **2017**, 147, 152715	3.9	22
223	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
222	A stress tensor eigenvector projection space for the (H2O)5 potential energy surface. *Chemical Physics Letters*, **2017**, 667, 25-31	2.5	19
221	Probing helical transitions in a DNA duplex. *Physical Chemistry Chemical Physics*, **2016**, 19, 878-892	3.6	18
220	Turning intractable counting into sampling: Computing the configurational entropy of three-dimensional jammed packings. *Physical Review E*, **2016**, 93, 012906	2.4	45
219	Kinetic Transition Networks for the Thomson Problem and Smale's Seventh Problem. *Physical Review Letters*, **2016**, 117, 028301	7.4	15
218	Energy landscapes for a machine-learning prediction of patient discharge. *Physical Review E*, **2016**, 93, 063310	2.4	14
217	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
216	GPU-Accelerated Exploration of Biomolecular Energy Landscapes. *Journal of Chemical Theory and Computation*, **2016**, 12, 6182-6191	6.4	15
215	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
214	Energy landscapes for a machine learning application to series data. *Journal of Chemical Physics*, **2016**, 144, 124119	3.9	19
213	Energetically favoured defects in dense packings of particles on spherical surfaces. *Soft Matter*, **2016**, 12, 5708-17	3.6	22
212	Rovibrational transitions of the methane-water dimer from intermolecular quantum dynamical computations. *Physical Chemistry Chemical Physics*, **2016**, 18, 22816-26	3.6	20
211	Structure and torsional dynamics of the water octamer from THz laser spectroscopy near 215 ℏ. *Science*, **2016**, 352, 1194-7	33.3	58
210	Grand and Semigrand Canonical Basin-Hopping. *Journal of Chemical Theory and Computation*, **2016**, 12, 902-9	6.4	21
209	Concerted hydrogen-bond breaking by quantum tunneling in the water hexamer prism. *Science*, **2016**, 351, 1310-3	33.3	182
208	Rate constants, timescales, and free energy barriers. *Journal of Non-Equilibrium Thermodynamics*, **2016**, 41,	3.8	11

207	Dynamical properties of two- and three-dimensional colloidal clusters of six particles. *Physical Chemistry Chemical Physics*, **2016**, 18, 12725-32	3.6	1
206	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
205	Dynamics of a molecular glass former: Energy landscapes for diffusion in ortho-terphenyl. *Journal of Chemical Physics*, **2016**, 145, 024505	3.9	23
204	Quantum tunneling splittings from path-integral molecular dynamics. *Journal of Chemical Physics*, **2016**, 144, 114108	3.9	24
203	Energy landscapes and persistent minima. *Journal of Chemical Physics*, **2016**, 144, 054109	3.9	8
202	Coarse-graining the structure of polycyclic aromatic hydrocarbons clusters. *Physical Chemistry Chemical Physics*, **2016**, 18, 13736-40	3.6	18
201	Conformational Energy Landscape of the Ritonavir Molecule. *Journal of Physical Chemistry B*, **2016**, 120, 4331-40	3.4	9
200	Self-assembly of colloidal magnetic particles: energy landscapes and structural transitions. *Physical Chemistry Chemical Physics*, **2016**, 18, 26579-26585	3.6	13
199	Structural analysis of high-dimensional basins of attraction. *Physical Review E*, **2016**, 94, 031301	2.4	12
198	QTAIM and stress tensor interpretation of the (H O) potential energy surface. *Journal of Computational Chemistry*, **2016**, 37, 2712-2721	3.5	8
197	Impurity effects on solid-solid transitions in atomic clusters. *Nanoscale*, **2016**, 8, 18326-18340	7.7	13
196	Potential energy landscapes of tetragonal pyramid molecules. *Chemical Physics Letters*, **2016**, 664, 5-9	2.5	3
195	The potential energy landscape for crystallisation of a Lennard-Jones fluid. *Journal of Statistical Mechanics: Theory and Experiment*, **2016**, 2016, 074001	1.9	10
194	Trapping of hydrogen atoms inside small beryllium clusters and their ions. *Chemical Physics Letters*, **2016**, 659, 282-288	2.5	0
193	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
192	Free energy basin-hopping. *Chemical Physics Letters*, **2015**, 625, 1-4	2.5	18
191	Membrane Protein Structure, Function, and Dynamics: a Perspective from Experiments and Theory. *Journal of Membrane Biology*, **2015**, 248, 611-40	2.3	101
190	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

189	Design of a Kagome lattice from soft anisotropic particles. *Soft Matter*, **2015**, 11, 6663-8	3.6	5
188	Exploring the potential energy landscape of the Thomson problem via Newton homotopies. *Journal of Chemical Physics*, **2015**, 142, 194113	3.9	9
187	Equilibrium molecular thermodynamics from Kirkwood sampling. *Journal of Physical Chemistry B*, **2015**, 119, 6155-69	3.4	1
186	Structures and Energy Landscapes of Hydrated Sulfate Clusters. *Journal of Chemical Theory and Computation*, **2015**, 11, 2377-84	6.4	27
185	Exploiting the potential energy landscape to sample free energy. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2015**, 5, 273-289	7.9	10
184	Quasi-combinatorial energy landscapes for nanoalloy structure optimisation. *Physical Chemistry Chemical Physics*, **2015**, 17, 28331-8	3.6	20
183	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
182	How to make a porphyrin flip: dynamics of asymmetric porphyrin oligomers. *Physical Chemistry Chemical Physics*, **2015**, 17, 27094-102	3.6	
181	Markov state modeling and dynamical coarse-graining via discrete relaxation path sampling. *Journal of Chemical Physics*, **2015**, 143, 044119	3.9	8
180	Computational investigation of RNA CUG repeats responsible for myotonic dystrophy 1. *Journal of Chemical Theory and Computation*, **2015**, 11, 4943-58	6.4	16
179	Intrinsically disordered energy landscapes. *Scientific Reports*, **2015**, 5, 10386	4.9	54
178	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	
177	Hydroxyproline Ring Pucker Causes Frustration of Helix Parameters in the Collagen Triple Helix. *Scientific Reports*, **2015**, 5, 12556	4.9	25
176	Perspective: Insight into reaction coordinates and dynamics from the potential energy landscape. *Journal of Chemical Physics*, **2015**, 142, 130901	3.9	66
175	Energy landscapes of a hairpin peptide including NMR chemical shift restraints. *Physical Chemistry Chemical Physics*, **2015**, 17, 20250-8	3.6	3
174	Chemistry, geometry, and defects in two dimensions. *ACS Nano*, **2014**, 8, 1081-5	16.7	13
173	A conformational factorisation approach for estimating the binding free energies of macromolecules. *Physical Chemistry Chemical Physics*, **2014**, 16, 2842-53	3.6	16
172	Exploring energy landscapes: from molecular to mesoscopic systems. *Physical Chemistry Chemical Physics*, **2014**, 16, 5014-25	3.6	15

171	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
170	An inversion-relaxation approach for sampling stationary points of spin model Hamiltonians. *Journal of Chemical Physics*, **2014**, 140, 194104	3.9	7
169	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
168	Energy landscapes of planar colloidal clusters. *Nanoscale*, **2014**, 6, 10717-26	7.7	18
167	Structure prediction for multicomponent materials using biminima. *Physical Review Letters*, **2014**, 113, 156102	7.4	20
166	Proton transfer pathways, energy landscape, and kinetics in creatine-water systems. *Journal of Physical Chemistry B*, **2014**, 118, 1969-75	3.4	5
165	Design principles for Bernal spirals and helices with tunable pitch. *Nanoscale*, **2014**, 6, 9448-56	7.7	23
164	Communication: Analysing kinetic transition networks for rare events. *Journal of Chemical Physics*, **2014**, 141, 041104	3.9	19
163	Communication: Newton homotopies for sampling stationary points of potential energy landscapes. *Journal of Chemical Physics*, **2014**, 141, 121104	3.9	13
162	Superposition Enhanced Nested Sampling. *Physical Review X*, **2014**, 4,	9.1	18
161	Communication: optimal parameters for basin-hopping global optimization based on Tsallis statistics. *Journal of Chemical Physics*, **2014**, 141, 071101	3.9	6
160	Certification and the potential energy landscape. *Journal of Chemical Physics*, **2014**, 140, 224114	3.9	5
159	Energy landscapes, folding mechanisms, and kinetics of RNA tetraloop hairpins. *Journal of the American Chemical Society*, **2014**, 136, 18052-61	16.4	37
158	Superposition-Enhanced Estimation of Optimal Temperature Spacings for Parallel Tempering Simulations. *Journal of Chemical Theory and Computation*, **2014**, 10, 5599-5605	6.4	8
157	A left-handed building block self-assembles into right- and left-handed helices. *RSC Advances*, **2013**, 3, 12905	3.7	14
156	Investigation of terahertz vibration-rotation tunneling spectra for the water octamer. *Journal of Physical Chemistry A*, **2013**, 117, 6960-6	2.8	44
155	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
154	Energy landscapes, structural topologies and rearrangement mechanisms in clusters of dipolar particles. *Soft Matter*, **2013**, 9, 5407	3.6	28

153	Symmetrisation schemes for global optimisation of atomic clusters. *Physical Chemistry Chemical Physics*, **2013**, 15, 3965-76	3.6	51
152	Surveying a complex potential energy landscape: Overcoming broken ergodicity using basin-sampling. *Chemical Physics Letters*, **2013**, 584, 1-9	2.5	51
151	Designing a Bernal spiral from patchy colloids. *ACS Nano*, **2013**, 7, 1246-56	16.7	35
150	Communication: Certifying the potential energy landscape. *Journal of Chemical Physics*, **2013**, 138, 171101	3.9	16
149	Visualizing basins of attraction for different minimization algorithms. *Journal of Physical Chemistry B*, **2013**, 117, 12717-23	3.4	34
148	Communication: a new paradigm for structure prediction in multicomponent systems. *Journal of Chemical Physics*, **2013**, 139, 221101	3.9	28
147	Energy landscapes and global thermodynamics for alanine peptides. *Journal of Chemical Physics*, **2013**, 139, 121909	3.9	19
146	Quasi-Continuous Interpolation Scheme for Pathways between Distant Configurations. *Journal of Chemical Theory and Computation*, **2012**, 8, 5020-34	6.4	27
145	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
144	A Local Rigid Body Framework for Global Optimization of Biomolecules. *Journal of Chemical Theory and Computation*, **2012**, 8, 5159-65	6.4	32
143	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
142	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
141	Beryllium cluster cages endohedrally doped by hydrogen: H2@Ben (8 □n □14). *International Journal of Quantum Chemistry*, **2012**, 112, 3068-3075	2.1	3
140	Decoding the energy landscape: extracting structure, dynamics and thermodynamics. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2012**, 370, 2877-99	3	58
139	Chemistry. Pinning down the water hexamer. *Science*, **2012**, 336, 814-5	33.3	57
138	Energy landscapes of colloidal clusters: thermodynamics and rearrangement mechanisms. *Nanoscale*, **2012**, 4, 1085-100	7.7	50
137	Chaotic dynamics near steep transition states. *Molecular Physics*, **2012**, 110, 1839-1848	1.7	4
136	Energy landscape and global optimization for a frustrated model protein. *Journal of Physical Chemistry B*, **2011**, 115, 11525-9	3.4	29

135	Coupled linear and rotary motion in supramolecular helix handedness inversion. *Soft Matter*, **2011**, 7, 2325	3.6	16
134	A survey of the potential energy surface for the (benzene)13 cluster. *Physical Chemistry Chemical Physics*, **2011**, 13, 21362-6	3.6	10
133	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
132	Instanton calculations of tunneling splittings for water dimer and trimer. *Journal of Chemical Physics*, **2011**, 135, 124109	3.9	65
131	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
130	Interpolation schemes for peptide rearrangements. *Journal of Chemical Physics*, **2010**, 132, 054101	3.9	13
129	Energy Landscapes and Structure Prediction Using Basin-Hopping **2010**, 29-54		5
128	The energy landscape, folding pathways and the kinetics of a knotted protein. *PLoS Computational Biology*, **2010**, 6, e1000835	5	37
127	Transmembrane structures for Alzheimer's A□(1-42) oligomers. *Journal of the American Chemical Society*, **2010**, 132, 13300-12	16.4	116
126	Emergent complexity from simple anisotropic building blocks: shells, tubes, and spirals. *ACS Nano*, **2010**, 4, 219-28	16.7	48
125	Energy landscapes: some new horizons. *Current Opinion in Structural Biology*, **2010**, 20, 3-10	8.1	116
124	Energy landscapes of clusters bound by short-ranged potentials. *ChemPhysChem*, **2010**, 11, 2491-4	3.2	58
123	Symmetrization of the AMBER and CHARMM force fields. *Journal of Computational Chemistry*, **2010**, 31, 1402-9	3.5	26
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