Ron Elber

List of Publications by Year in Descending Order

168 papers	8,651 citations	46 h-index	90 g-index
181 ext. papers	9,450 ext. citations	5.1 avg, IF	6.39 L-index

#	Paper	IF	Citations
168	Computer Simulations of the Dissociation Mechanism of Gleevec from Abl Kinase with Milestoning. *Journal of Physical Chemistry B*, **2021**, 125, 5706-5715	3.4	8
167	Catalytic Magnesium as a Door Stop for DNA Sliding. *Journal of Physical Chemistry B*, **2021**, 125, 3494-3500	3.4	0
166	Modeling molecular kinetics with Milestoning. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1512	7.9	1
165	Interfacial Dynamics in Lipid Membranes: The Effects of Headgroup Structures. *Journal of Physical Chemistry B*, **2021**, 125, 1343-1350	3.4	7
164	Impact of the Protonation State of Phosphatidylinositol 4,5-Bisphosphate (PIP2) on the Binding Kinetics and Thermodynamics to Transient Receptor Potential Vanilloid (TRPV5): A Milestoning Study. *Journal of Physical Chemistry B*, **2021**, 125, 9547-9556	3.4	2
163	Exploring the Reaction Mechanism of HIV Reverse Transcriptase with a Nucleotide Substrate. *Journal of Physical Chemistry B*, **2020**, 124, 4270-4283	3.4	5
162	Simple and Analytical Model of RNA Collapse. *Journal of Physical Chemistry B*, **2020**, 124, 5149-5155	3.4	
161	Milestoning: An Efficient Approach for Atomically Detailed Simulations of Kinetics in Biophysics. *Annual Review of Biophysics*, **2020**, 49, 69-85	21.1	15
160	Phase Transition in a Heterogeneous Membrane: Atomically Detailed Picture. *Journal of Physical Chemistry Letters*, **2020**, 11, 5263-5267	6.4	2
159	Milestoning with wind: Exploring the impact of a biasing potential in exact calculation of kinetics. *Journal of Chemical Physics*, **2020**, 152, 224105	3.9	2
158	Calcium-Lipid Interactions Observed with Isotope-Edited Infrared Spectroscopy. *Biophysical Journal* , **2020**, 118, 2694-2702	2.9	5
157	Long-time methods for molecular dynamics simulations: Markov State Models and Milestoning. *Progress in Molecular Biology and Translational Science*, **2020**, 170, 215-237	4	6
156	**2020**,		15
155	The Schrdinger Representation **2020**, 41-47		
154	A Simple Numerical Example of Rate Calculations **2020**, 223-231		
153	Path Integrals **2020**, 63-67		
152	Rare Events and Reaction Coordinates **2020**, 233-240		

151 The Master Equation as a Model for Transitions Between Macrostates **2020**, 203-212

150 Barrier Crossing **2020**, 69-87

149 An Example of the Use of Cells **2020**, 255-257

148 The Rate of Conformational Change **2020**, 117-131

147 Zwanzig-Caldeiga-Leggett Model for Low-Dimensional Dynamics **2020**, 133-145

146 The FokkerPlanck Equation **2020**, 29-39

145 Escape from a Potential Well in the Case of Dynamics Obeying the Generalized Langevin Equation **2020**, 147-156

144 Computer Simulations of Molecular Kinetics **2020**, 193-202

143 Discrete Systems **2020**, 49-61

142 Quantum Effects in Chemical Kinetics **2020**, 173-191

141 Celling **2020**, 241-253

140 Direct Calculation of Rate Coefficients with Computer Simulations **2020**, 213-221

139 The Langevin Equation and Stochastic Processes **2020**, 1-27

138 Diffusive Dynamics on a Multidimensional Energy Landscape **2020**, 157-171

137 Sampling Transition Paths **2020**, 89-115

136 ScMile: A Script to Investigate Kinetics with Short Time Molecular Dynamics Trajectories and the Milestoning Theory. *Journal of Chemical Theory and Computation*, **2020**, 16, 860-874 6.4 2

135 The transition between active and inactive conformations of Abl kinase studied by rock climbing and Milestoning. *Biochimica Et Biophysica Acta - General Subjects*, **2020**, 1864, 129508 4 11

134 Computer simulations of a heterogeneous membrane with enhanced sampling techniques. *Journal of Chemical Physics*, **2020**, 153, 144110 3.9 5

133	Dramatic Shape Changes Occur as Cytochrome Folds. *Journal of Physical Chemistry B*, **2020**, 124, 8240-8248	3.4	2
132	Value of Temporal Information When Analyzing Reaction Coordinates. *Journal of Chemical Theory and Computation*, **2020**, 16, 6077-6090	6.4	3
131	Partition of Positively and Negatively Charged Tryptophan Ions in Membranes with Inverted Phospholipid Heads: Simulations and Experiments. *Journal of Physical Chemistry B*, **2019**, 123, 3272-3281	3.4	2
130	Defect-Assisted Permeation Through a Phospholipid Membrane: Experimental and Computational Study of the Peptide WKW. *Journal of Physical Chemistry B*, **2019**, 123, 6792-6798	3.4	3
129	Preferential Equilibrium Partitioning of Positively Charged Tryptophan into Phosphatidylcholine Bilayer Membranes. *Journal of Physical Chemistry B*, **2019**, 123, 170-179	3.4	7
128	Conformations of an RNA Helix-Junction-Helix Construct Revealed by SAXS Refinement of MD Simulations. *Biophysical Journal*, **2019**, 116, 19-30	2.9	9
127	Ion Permeation through a Phospholipid Membrane: Transition State, Path Splitting, and Calculation of Permeability. *Journal of Chemical Theory and Computation*, **2019**, 15, 720-730	6.4	14
126	Why Does RNA Collapse? The Importance of Water in a Simulation Study of Helix-Junction-Helix Systems. *Journal of the American Chemical Society*, **2018**, 140, 16948-16951	16.4	13
125	Physiological Calcium Concentrations Slow Dynamics at the Lipid-Water Interface. *Biophysical Journal*, **2018**, 115, 1541-1551	2.9	16
124	Probing Translocation in Mutants of the Anthrax Channel: Atomically Detailed Simulations with Milestoning. *Journal of Physical Chemistry B*, **2018**, 122, 10296-10305	3.4	4
123	Revealing the distinct folding phases of an RNA three-helix junction. *Nucleic Acids Research*, **2018**, 46, 7354-7365	20.1	23
122	A mixed alchemical and equilibrium dynamics to simulate heterogeneous dense fluids: Illustrations for Lennard-Jones mixtures and phospholipid membranes. *Journal of Chemical Physics*, **2018**, 149, 072325	3.9	9
121	Direct Measurement of the Effect of Cholesterol and 6-Ketocholestanol on the Membrane Dipole Electric Field Using Vibrational Stark Effect Spectroscopy Coupled with Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2017**, 121, 3424-3436	3.4	12
120	A new paradigm for atomically detailed simulations of kinetics in biophysical systems. *Quarterly Reviews of Biophysics*, **2017**, 50, e8	7	37
119	The Impact of Protonation on Early Translocation of Anthrax Lethal Factor: Kinetics from Molecular Dynamics Simulations and Milestoning Theory. *Journal of the American Chemical Society*, **2017**, 139, 14837-14840	16.4	22
118	Rock climbing: A local-global algorithm to compute minimum energy and minimum free energy pathways. *Journal of Chemical Physics*, **2017**, 147, 152718	3.9	7
117	Pyrophosphate Release in the Protein HIV Reverse Transcriptase. *Journal of Physical Chemistry B*, **2017**, 121, 9557-9565	3.4	11
116	Calculating Iso-Committor Surfaces as Optimal Reaction Coordinates with Milestoning. *Entropy*, **2017**, 19,	2.8	30

115	A MATHEMATICAL FRAMEWORK FOR EXACT MILESTONING. *Multiscale Modeling and Simulation*, **2016**, 14, 301-322	1.8	13
114	Prediction of homoprotein and heteroprotein complexes by protein docking and template-based modeling: A CASP-CAPRI experiment. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84 Suppl 1, 323-48	4.2	111
113	Simulations of thermodynamics and kinetics on rough energy landscapes with milestoning. *Journal of Computational Chemistry*, **2016**, 37, 602-13	3.5	9
112	Perspective: Computer simulations of long time dynamics. *Journal of Chemical Physics*, **2016**, 144, 060901	3.9	46
111	Markovian and Non-Markovian Modeling of Membrane Dynamics with Milestoning. *Journal of Physical Chemistry B*, **2016**, 120, 8208-16	3.4	12
110	Comprehensive analysis of sequences of a protein switch. *Protein Science*, **2016**, 25, 135-46	6.3	11
109	From an SNP to a Disease: A Comprehensive Statistical Analysis. *Structure*, **2015**, 23, 1155	5.2	1
108	Molecular dynamics studies of modular polyketide synthase ketoreductase stereospecificity. *Biochemistry*, **2015**, 54, 2346-59	3.2	14
107	Membrane permeation of a peptide: it is better to be positive. *Journal of Physical Chemistry B*, **2015** , 119, 6412-20	3.4	32
106	Enzyme Selectivity of HIV Reverse Transcriptase: Conformations, Ligands, and Free Energy Partition. *Journal of Physical Chemistry B*, **2015**, 119, 11513-26	3.4	24
105	Extracting the diffusion tensor from molecular dynamics simulation with Milestoning. *Journal of Chemical Physics*, **2015**, 142, 014105	3.9	12
104	A Stochastic Algorithm for the Isobaric-Isothermal Ensemble with Ewald Summations for All Long Range Forces. *Journal of Chemical Theory and Computation*, **2015**, 11, 5624-37	6.4	48
103	Exact milestoning. *Journal of Chemical Physics*, **2015**, 142, 094102	3.9	78
102	Extension of a protein docking algorithm to membranes and applications to amyloid precursor protein dimerization. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 2170-85	4.2	11
101	Measurement of the membrane dipole electric field in DMPC vesicles using vibrational shifts of p-cyanophenylalanine and molecular dynamics simulations. *Journal of Physical Chemistry B*, **2015**, 119, 2869-76	3.4	22
100	Two is a pair, three is a network. *Biophysical Journal*, **2015**, 108, 22	2.9	
99	The energy landscape of a protein switch. *Physical Chemistry Chemical Physics*, **2014**, 16, 6407-21	3.6	12
98	Modeling kinetics and equilibrium of membranes with fields: milestoning analysis and implication to permeation. *Journal of Chemical Physics*, **2014**, 141, 054101	3.9	30

97	Molecular Dynamics at Extended Timescales. *Israel Journal of Chemistry*, **2014**, 54, 1302-1310	3.4	1
96	DOCK/PIERR: web server for structure prediction of protein-protein complexes. *Methods in Molecular Biology*, **2014**, 1137, 199-207	1.4	26
95	Computational study of peptide permeation through membrane: Searching for hidden slow variables. *Molecular Physics*, **2013**, 111, 3565-3578	1.7	31
94	Coiled-coil response to mechanical force: global stability and local cracking. *Biophysical Journal*, **2013**, 105, 951-61	2.9	16
93	Molecular machines. *Current Opinion in Structural Biology*, **2013**, 23, 206-11	8.1	8
92	Improving ranking of models for protein complexes with side chain modeling and atomic potentials. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 592-606	4.2	37
91	Catch bond-like kinetics of helix cracking: network analysis by molecular dynamics and milestoning. *Journal of Chemical Physics*, **2013**, 139, 121902	3.9	23
90	Analyzing milestoning networks for molecular kinetics: definitions, algorithms, and examples. *Journal of Chemical Physics*, **2013**, 139, 174105	3.9	17
89	How conformational dynamics of DNA polymerase select correct substrates: experiments and simulations. *Structure*, **2012**, 20, 618-27	5.2	91
88	9.2 Coarse-Grained Methods: Theory **2012**, 2-26		1
87	Experiments and comprehensive simulations of the formation of a helical turn. *Journal of Physical Chemistry B*, **2012**, 116, 6598-610	3.4	20
86	Revisiting Molecular Dynamics on a CPU/GPU system: Water Kernel and SHAKE Parallelization. *Journal of Chemical Theory and Computation*, **2012**, 8, 4624-4636	6.4	18
85	Early events in helix unfolding under external forces: a milestoning analysis. *Journal of Physical Chemistry B*, **2012**, 116, 8662-91	3.4	19
84	Thermodynamic Cycle Without Turning Off Self-Interactions: Formal Discussion and a Numerical Example. *Journal of Chemical Theory and Computation*, **2012**, 8, 3022-3033	6.4	7
83	The ionic atmosphere around A-RNA: Poisson-Boltzmann and molecular dynamics simulations. *Biophysical Journal*, **2012**, 102, 829-38	2.9	57
82	RNA and its ionic cloud: solution scattering experiments and atomically detailed simulations. *Biophysical Journal*, **2012**, 102, 819-28	2.9	75
81	Chapter 6:Enhancing the Capacity of Molecular Dynamics Simulations with Trajectory Fragments. *RSC Biomolecular Sciences*, **2012**, 117-137		1
80	Super folds, networks, and barriers. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 463-70	4.2	11

79	Unassisted transport of N-acetyl-L-tryptophanamide through membrane: experiment and simulation of kinetics. *Journal of Physical Chemistry B*, **2012**, 116, 2739-50	3.4	51
78	Dynamics of induced-fit in HIV reverse transcriptase specificity and resistance. *FASEB Journal*, **2012**, 26, 964.5	0.9	
77	MOIL-opt: Energy-Conserving Molecular Dynamics on a GPU/CPU system. *Journal of Chemical Theory and Computation*, **2011**, 7, 3072-3082	6.4	42
76	Progress at last. *Structure*, **2011**, 19, 1725	5.2	1
75	Simulations of allosteric transitions. *Current Opinion in Structural Biology*, **2011**, 21, 167-72	8.1	35
74	SHAKE parallelization. *European Physical Journal: Special Topics*, **2011**, 200, 211-223	2.3	36
73	Revisiting and computing reaction coordinates with Directional Milestoning. *Journal of Physical Chemistry A*, **2011**, 115, 6137-48	2.8	61
72	Energy design for protein-protein interactions. *Journal of Chemical Physics*, **2011**, 135, 065102	3.9	12
71	Atomically detailed simulation of the recovery stroke in myosin by Milestoning. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 5001-5	11.5	58
70	Milestoning without a Reaction Coordinate. *Journal of Chemical Theory and Computation*, **2010**, 6, 1805-1817	5.4	89
69	Ligand diffusion in globins: simulations versus experiment. *Current Opinion in Structural Biology*, **2010**, 20, 162-7	8.1	72
68	Watching biomolecular machines in action. *Structure*, **2010**, 18, 415-6	5.2	0
67	PIE-efficient filters and coarse grained potentials for unbound protein-protein docking. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 400-19	4.2	39
66	Computational exploration of the network of sequence flow between protein structures. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 985-1003	4.2	19
65	A coarse-grained potential for fold recognition and molecular dynamics simulations of proteins. *Proteins: Structure, Function and Bioinformatics*, **2009**, 76, 822-36	4.2	43
64	Building and assessing atomic models of proteins from structural templates: learning and benchmarks. *Proteins: Structure, Function and Bioinformatics*, **2009**, 76, 930-45	4.2	23
63	Kinetics of helix unfolding: molecular dynamics simulations with milestoning. *Journal of Physical Chemistry A*, **2009**, 113, 7461-73	2.8	57
62	Toward quantitative simulations of carbon monoxide escape pathways in myoglobin. *Journal of Physical Chemistry B*, **2008**, 112, 6147-54	3.4	32

61	On the assumptions underlying milestoning. *Journal of Chemical Physics*, **2008**, 129, 174102	3.9	138
60	A template-finding algorithm and a comprehensive benchmark for homology modeling of proteins. *Proteins: Structure, Function and Bioinformatics*, **2008**, 72, 910-28	4.2	17
59	Extending molecular dynamics time scales with milestoning: example of complex kinetics in a solvated peptide. *Journal of Chemical Physics*, **2007**, 126, 145104	3.9	140
58	A milestoning study of the kinetics of an allosteric transition: atomically detailed simulations of deoxy Scapharca hemoglobin. *Biophysical Journal*, **2007**, 92, L85-7	2.9	83
57	The network of sequence flow between protein structures. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 11627-32	11.5	40
56	Calculation of Point-to-Point Short-Time and Rare Trajectories with Boundary Value Formulation. *Journal of Chemical Theory and Computation*, **2006**, 2, 484-94	6.4	19
55	SSALN: an alignment algorithm using structure-dependent substitution matrices and gap penalties learned from structurally aligned protein pairs. *Proteins: Structure, Function and Bioinformatics*, **2006**, 62, 881-91	4.2	68
54	Revisiting and parallelizing SHAKE. *Journal of Computational Physics*, **2005**, 209, 193-206	4.1	55
53	Long-timescale simulation methods. *Current Opinion in Structural Biology*, **2005**, 15, 151-6	8.1	145
52	Atomically detailed potentials to recognize native and approximate protein structures. *Proteins: Structure, Function and Bioinformatics*, **2005**, 61, 44-55	4.2	38
51	Computing time scales from reaction coordinates by milestoning. *Journal of Chemical Physics*, **2004**, 120, 10880-9	3.9	476
50	The evolutionary capacity of protein structures **2004**,		6
49	Computational analysis of sequence selection mechanisms. *Structure*, **2004**, 12, 547-57	5.2	15
48	Large-scale linear programming techniques for the design of protein folding potentials. *Mathematical Programming*, **2004**, 101, 301	2.1	17
47	Enriching the sequence substitution matrix by structural information. *Proteins: Structure, Function and Bioinformatics*, **2004**, 54, 41-8	4.2	78
46	Bridging the Gap between Long Time Trajectories and Reaction Pathways. *Advances in Chemical Physics*, **2003**, 93-129		27
45	Kinetics of cytochrome C folding: atomically detailed simulations. *Proteins: Structure, Function and Bioinformatics*, **2003**, 51, 245-57	4.2	52
44	Maximum feasibility guideline in the design and analysis of protein folding potentials. *Journal of Computational Chemistry*, **2002**, 23, 111-8	3.5	21

43	An atomically detailed study of the folding pathways of protein A with the stochastic difference equation. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 10394-8	11.5	119
42	Long time dynamics of complex systems. *Accounts of Chemical Research*, **2002**, 35, 396-403	24.3	96
41	Protein Recognition by Sequence-to-Structure Fitness: Bridging Efficiency and Capacity of Threading Models. *Advances in Chemical Physics*, **2002**, 77-130		4
40	Enzymatic circularization of a malto-octaose linear chain studied by stochastic reaction path calculations on cyclodextrin glycosyltransferase. *Proteins: Structure, Function and Bioinformatics*, **2001**, 43, 327-35	4.2	31
39	Linear programming optimization and a double statistical filter for protein threading protocols. *Proteins: Structure, Function and Bioinformatics*, **2001**, 45, 241-61	4.2	113
38	On the design and analysis of protein folding potentials. *Proteins: Structure, Function and Bioinformatics*, **2000**, 40, 71-85	4.2	100
37	Distance-dependent, pair potential for protein folding: Results from linear optimization. *Proteins: Structure, Function and Bioinformatics*, **2000**, 41, 40-46	4.2	155
36	Probing the role of local propensity in peptide turn formation. *International Journal of Quantum Chemistry*, **2000**, 80, 1125-1128	2.1	3
35	Temperature dependent reaction coordinates. *Journal of Chemical Physics*, **2000**, 112, 5539-5545	3.9	66
34	fw2.2: a quantitative trait locus key to the evolution of tomato fruit size. *Science*, **2000**, 289, 85-8	33.3	1084
33	Chemical Development of Latent Fingerprints: Computational Design of Ninhydrin Analogues. *Journal of Forensic Sciences*, **2000**, 45, 14767J	1.8	20
32	Chemical development of latent fingerprints: computational design of ninhydrin analogues. *Journal of Forensic Sciences*, **2000**, 45, 757-60	1.8	1
31	Distance-dependent, pair potential for protein folding: results from linear optimization. *Proteins: Structure, Function and Bioinformatics*, **2000**, 41, 40-6	4.2	57
30	Unit-vector RMS (URMS) as a tool to analyze molecular dynamics trajectories. *Proteins: Structure, Function and Bioinformatics*, **1999**, 37, 554-564	4.2	41
29	Stochastic Path Approach to Compute Atomically Detailed Trajectories: Application to the Folding of C Peptide. *Journal of Physical Chemistry B*, **1999**, 103, 899-911	3.4	96
28	Unit-vector RMS (URMS) as a tool to analyze molecular dynamics trajectories **1999**, 37, 554		1
27	Unit-vector RMS (URMS) as a tool to analyze molecular dynamics trajectories **1999**, 37, 554		1
26	Yet another look at the steepest descent path. *Computational and Theoretical Chemistry*, **1997**, 398-399, 63-71		68

25	Calculation of classical trajectories with a very large time step: Formalism and numerical examples. *Journal of Chemical Physics*, **1996**, 105, 9299-9315	3.9	182
24	REACTION PATH STUDIES OF BIOLOGICAL MOLECULES. *Advanced Series in Physical Chemistry*, **1996**, 65-136		7
23	Homology as a Tool in Optimization Problems: Structure Determination of 2D Heteropolymers. *The Journal of Physical Chemistry*, **1995**, 99, 11550-11556		13
22	Computer determination of peptide conformations in water: different roads to structure. *Proceedings of the National Academy of Sciences of the United States of America*, **1995**, 92, 3190-3	11.5	31
21	Sodium in gramicidin: an example of a permion. *Biophysical Journal*, **1995**, 68, 906-24	2.9	62
20	MOIL: A program for simulations of macromolecules. *Computer Physics Communications*, **1995**, 91, 159-189	4.2	145
19	The thermal equilibrium aspects of the time dependent Hartree and the locally enhanced sampling approximations: Formal properties, a correction, and computational examples for rare gas clusters. *Journal of Chemical Physics*, **1993**, 98, 3380-3388	3.9	38
18	Ligand binding and conformation change in the dimeric hemoglobin of the clam Scapharca inaequivalvis. *Journal of Biological Chemistry*, **1993**, 268, 5711-8	5.4	25
17	Ligand binding and conformation change in the dimeric hemoglobin of the clam Scapharca inaequivalvis.. *Journal of Biological Chemistry*, **1993**, 268, 5711-5718	5.4	28
16	Locally enhanced sampling in free energy calculations: Application of mean field approximation to accurate calculation of free energy differences. *Journal of Chemical Physics*, **1992**, 97, 7838-7841	3.9	44
15	Computational studies of ligand diffusion in globins: I. Leghemoglobin. *Proteins: Structure, Function and Bioinformatics*, **1991**, 10, 70-80	4.2	64
14	Reaction path study of helix formation in tetrapeptides: Effect of side chains. *Journal of Chemical Physics*, **1991**, 94, 751-760	3.9	115
13	Modeling side chains in peptides and proteins: Application of the locally enhanced sampling and the simulated annealing methods to find minimum energy conformations. *Journal of Chemical Physics*, **1991**, 95, 9277-9287	3.9	159
12	Molecular dynamics study of secondary structure motions in proteins: application to myohemerythrin. *Proteins: Structure, Function and Bioinformatics*, **1990**, 7, 265-79	4.2	28
11	Self-avoiding walk between two fixed points as a tool to calculate reaction paths in large molecular systems. *International Journal of Quantum Chemistry*, **1990**, 38, 167-185	2.1	115
10	A new technique to calculate steepest descent paths in flexible polyatomic systems. *Journal of Chemical Physics*, **1990**, 92, 1510-1511	3.9	242
9	Calculation of the potential of mean force using molecular dynamics with linear constraints: An application to a conformational transition in a solvated dipeptide. *Journal of Chemical Physics*, **1990**, 93, 4312-4321	3.9	61
8	Enhanced sampling in molecular dynamics: use of the time-dependent Hartree approximation for a simulation of carbon monoxide diffusion through myoglobin. *Journal of the American Chemical Society*, **1990**, 112, 9161-9175	16.4	475

7	Reaction path study of conformational transitions in flexible systems: Applications to peptides. *Journal of Chemical Physics*, **1990**, 92, 5580-5601	3.9	234
6	Calculations of a list of neighbors in Molecular Dynamics simulations. *Journal of Computational Chemistry*, **1989**, 10, 921-927	3.5	29
5	Reaction path study of conformational transitions and helix formation in a tetrapeptide. *Proceedings of the National Academy of Sciences of the United States of America*, **1989**, 86, 6963-7	11.5	60
4	A method for determining reaction paths in large molecules: Application to myoglobin. *Chemical Physics Letters*, **1987**, 139, 375-380	2.5	353
3	Multiple conformational states of proteins: a molecular dynamics analysis of myoglobin. *Science*, **1987**, 235, 318-21	33.3	617
2	Lifetimes of rotational resonances in molecule-surface scattering. *Molecular Physics*, **1985**, 55, 1369-1381	1.7	26
1	A new boundary driven NEMD scheme for heat and particle diffusion in binary mixtures. *Molecular Physics*,e1892849	1.7	0