Rigoberto Hernandez

List of Publications by Year
in descending order

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162 papers	3,660 citations	126858 33 h-index	175177 52 g-index
170 all docs	170 docs citations	170 times ranked	2280 citing authors

#	Article	IF	Citations
1	Ab initio calculation of anharmonic constants for a transition state, with application to semiclassical transition state tunneling probabilities. Chemical Physics Letters, 1990, 172, 62-68.	1.2	221
2	Semiclassical transition state theory. A new perspective. Chemical Physics Letters, 1993, 214, 129-136.	1.2	180
3	A transition state theoryâ€based statistical distribution of unimolecular decay rates with application to unimolecular decomposition of formaldehyde. Journal of Chemical Physics, 1990, 93, 5657-5666.	1.2	128
4	Biological Responses to Engineered Nanomaterials: Needs for the Next Decade. ACS Central Science, 2015, 1, 117-123.	5.3	121
5	Adaptive Steered Molecular Dynamics of the Long-Distance Unfolding of Neuropeptide Y. Journal of Chemical Theory and Computation, 2010, 6, 3026-3038.	2.3	88
6	Mechanism for Radical Cation Transport in Duplex DNA Oligonucleotides. Journal of the American Chemical Society, 2004, 126, 2877-2884.	6.6	84
7	Transition State in a Noisy Environment. Physical Review Letters, 2005, 95, 058301.	2.9	75
8	Adaptive steered molecular dynamics: Validation of the selection criterion and benchmarking energetics in vacuum. Journal of Chemical Physics, 2012, 136, 215104.	1.2	72
9	On the accuracy limits of orbital expansion methods: Explicit effects ofk-functions on atomic and molecular energies. Journal of Chemical Physics, 2003, 118, 8594-8610.	1.2	70
10	Transition state theory in liquids beyond planar dividing surfaces. Chemical Physics, 2010, 370, 270-276.	0.9	68
11	Lagrangian Descriptors of Thermalized Transition States on Time-Varying Energy Surfaces. Physical Review Letters, 2015, 115, 148301.	2.9	68
12	Cumulative reaction probabilities for H+H2â†'H2+H from a knowledge of the anharmonic force field. Chemical Physics Letters, 1992, 192, 407-416.	1.2	67
13	Solution NMR Analysis of Ligand Environment in Quaternary Ammonium-Terminated Self-Assembled Monolayers on Gold Nanoparticles: The Effect of Surface Curvature and Ligand Structure. Journal of the American Chemical Society, 2019, 141, 4316-4327.	6.6	66
14	Quantum time correlation functions and classical coherence. Chemical Physics, 1998, 233, 243-255.	0.9	65
15	Probing the Cybotactic Region in Gas-Expanded Liquids (GXLs). Accounts of Chemical Research, 2006, 39, 531-538.	7.6	65
16	Stochastic transition states: Reaction geometry amidst noise. Journal of Chemical Physics, 2005, 123, 204102.	1.2	57
17	A combined use of perturbation theory and diagonalization: Application to bound energy levels and semiclassical rate theory. Journal of Chemical Physics, 1994, 101, 9534-9547.	1.2	56
18	A random matrix/transition state theory for the probability distribution of stateâ€specific unimolecular decay rates: Generalization to include total angular momentum conservation and other dynamical symmetries. Journal of Chemical Physics, 1993, 99, 950-962.	1.2	53

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19	Thermodynamics of Decaalanine Stretching in Water Obtained by Adaptive Steered Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2012, 8, 4837-4844.	2.3	52
20	Sustainable Nanotechnology: Opportunities and Challenges for Theoretical/Computational Studies. Journal of Physical Chemistry B, 2016, 120, 7297-7306.	1.2	52
21	Stochastic Dynamics in Irreversible Nonequilibrium Environments. 1. The Fluctuationâ^'Dissipation Relation. Journal of Physical Chemistry B, 1999, 103, 1064-1069.	1.2	49
22	Deconstructing field-induced ketene isomerization through Lagrangian descriptors. Physical Chemistry Chemical Physics, 2016, 18, 4008-4018.	1.3	49
23	Identifying reactive trajectories using a moving transition state. Journal of Chemical Physics, 2006, 124, 244310.	1.2	47
24	Lipid Corona Formation from Nanoparticle Interactions with Bilayers. CheM, 2018, 4, 2709-2723.	5.8	46
25	Multiple branched adaptive steered molecular dynamics. Journal of Chemical Physics, 2014, 141, 064101.	1.2	43
26	Solvent-Induced Acceleration of the Rate of Activation of a Molecular Reaction. Physical Review Letters, 2008, 101, 178302.	2.9	40
27	The projection of a mechanical system onto the irreversible generalized Langevin equation. Journal of Chemical Physics, 1999, 111, 7701-7704.	1.2	39
28	Transition state geometry of driven chemical reactions on time-dependent double-well potentials. Physical Chemistry Chemical Physics, 2016, 18, 30270-30281.	1.3	37
29	Molecular Dynamics Simulation of the Cybotactic Region in Gas-Expanded Methanolâ^'Carbon Dioxide and Acetoneâ^'Carbon Dioxide Mixtures. Journal of Physical Chemistry B, 2006, 110, 24101-24111.	1.2	36
30	Uncovering the Geometry of Barrierless Reactions Using Lagrangian Descriptors. Journal of Physical Chemistry B, 2016, 120, 1720-1725.	1.2	35
31	Lagrangian descriptors of driven chemical reaction manifolds. Physical Review E, 2017, 96, 022222.	0.8	35
32	Diffusional effects on the reversible excited-state proton transfer. From experiments to Brownian dynamics simulations. Physical Chemistry Chemical Physics, 2011, 13, 14914.	1.3	34
33	Ontology of temperature in nonequilibrium systems. Journal of Chemical Physics, 2007, 126, 244506.	1.2	33
34	Constrained Unfolding of a Helical Peptide: Implicit versus Explicit Solvents. PLoS ONE, 2015, 10, e0127034.	1.1	33
35	Obtaining time-dependent multi-dimensional dividing surfaces using Lagrangian descriptors. Chemical Physics Letters, 2017, 687, 194-199.	1.2	33
36	Using an environmentally-relevant panel of Gram-negative bacteria to assess the toxicity of polyallylamine hydrochloride-wrapped gold nanoparticles. Environmental Science: Nano, 2018, 5, 279-288.	2.2	32

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37	Stochastic Dynamics in Irreversible Nonequilibrium Environments. 2. A Model for Thermosetting Polymerization. Journal of Physical Chemistry B, 1999, 103, 1070-1077.	1.2	31
38	Preferential Binding of Cytochrome c to Anionic Ligand-Coated Gold Nanoparticles: A Complementary Computational and Experimental Approach. ACS Nano, 2019, 13, 6856-6866.	7.3	31
39	Femtosecond-Laser Desorption of H₂ (D₂) from Ru(0001): Quantum and Classical Approaches. Journal of Physical Chemistry C, 2009, 113, 7790-7801.	1.5	30
40	Chemical dynamics between wells across a time-dependent barrier: Self-similarity in the Lagrangian descriptor and reactive basins. Journal of Chemical Physics, 2017, 147, 064101.	1.2	29
41	Chemical reactions induced by oscillating external fields in weak thermal environments. Journal of Chemical Physics, 2015, 142, 074108.	1.2	28
42	Communication: Transition state trajectory stability determines barrier crossing rates in chemical reactions induced by time-dependent oscillating fields. Journal of Chemical Physics, 2014, 141, 041106.	1.2	27
43	Effects of Roaming Trajectories on the Transition State Theory Rates of a Reduced-Dimensional Model of Ketene Isomerization. Journal of Physical Chemistry A, 2013, 117, 7553-7560.	1.1	24
44	Peripheral Membrane Proteins Facilitate Nanoparticle Binding at Lipid Bilayer Interfaces. Langmuir, 2018, 34, 10793-10805.	1.6	24
45	Important fluctuation dynamics of large protein structures are preserved upon coarse-grained renormalization. International Journal of Quantum Chemistry, 2002, 90, 822-837.	1.0	23
46	A Spectroscopic and Computational Exploration of the Cybotactic Region of Gas-Expanded Liquids:â€‰ Methanol and Acetone. Journal of Physical Chemistry B, 2008, 112, 4666-4673.	1.2	23
47	Persistence of transition-state structure in chemical reactions driven by fields oscillating in time. Physical Review E, 2014, 89, 040801.	0.8	23
48	Density, Structure, and Stability of Citrate^{3â€“} and H₂citrate^{â€“} on Bare and Coated Gold Nanoparticles. Journal of Physical Chemistry C, 2018, 122, 28393-28404.	1.5	23
49	Invariant Manifolds and Rate Constants in Driven Chemical Reactions. Journal of Physical Chemistry B, 2019, 123, 2070-2086.	1.2	23
50	Transition-State Theory Rate Calculations with a Recrossing-Free Moving Dividing Surface. Journal of Physical Chemistry B, 2008, 112, 206-212.	1.2	22
51	Dynamical simulation of dipolar Janus colloids: Equilibrium structure and thermodynamics. Journal of Chemical Physics, 2012, 137, 044505.	1.2	22
52	Determining the Energetics of Small Î²-Sheet Peptides using Adaptive Steered Molecular Dynamics. Journal of Chemical Theory and Computation, 2016, 12, 2028-2037.	2.3	22
53	Chemical reaction dynamics within anisotropic solvents in time-dependent fields. Journal of Chemical Physics, 2005, 122, 014509.	1.2	21
54	Adsorption Dynamics and Structure of Polycations on Citrate-Coated Gold Nanoparticles. Journal of Physical Chemistry C, 2018, 122, 19962-19969.	1.5	21

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55	Chemical reaction dynamics with stochastic potentials below the high-friction limit. Journal of Chemical Physics, 2001, 115, 2430-2438.	1.2	20
56	Dynamics of Swelling/Contracting Hard Spheres Surmised by an Irreversible Langevin Equationâ€. Journal of Physical Chemistry A, 2006, 110, 1635-1644.	1.1	19
57	Transition state theory for activated systems with driven anharmonic barriers. Journal of Chemical Physics, 2017, 147, 074104.	1.2	19
58	Binary contraction method for the construction of time-dependent dividing surfaces in driven chemical reactions. Physical Review E, 2018, 98, .	0.8	19
59	A minimalist model protein with multiple folding funnels. Proceedings of the National Academy of Sciences of the United States of America, 2001, 98, 9074-9079.	3.3	18
60	Detailed study of the direct numerical observation of the Kramers turnover in the LiNCâ‡ŒLiCN isomerization rate. Journal of Chemical Physics, 2012, 137, 204301.	1.2	18
61	On the Feynman path centroid density as a phase space distribution in quantum statistical mechanics. Journal of Chemical Physics, 1995, 103, 5018-5026.	1.2	17
62	Stochastic Dynamics in Irreversible Nonequilibrium Environments. 4. Self-Consistent Coupling in Heterogeneous Environments. Journal of Physical Chemistry B, 2000, 104, 3456-3462.	1.2	17
63	Observation of a Trapping Transition in the Diffusion of a Thick Needle through Fixed Point Scatterers. Journal of Physical Chemistry A, 2010, 114, 9628-9634.	1.1	17
64	Lagrangian descriptors in dissipative systems. Physical Chemistry Chemical Physics, 2016, 18, 30282-30287.	1.3	16
65	Adaptive steered molecular dynamics of biomolecules. Molecular Simulation, 2021, 47, 408-419.	0.9	16
66	The Middle Science: Traversing Scale In Complex Many-Body Systems. ACS Central Science, 2021, 7, 1271-1287.	5.3	16
67	Stochastic Dynamics in Irreversible Nonequilibrium Environments. 3. Temperature-Ramped Chemical Kinetics. Journal of Physical Chemistry A, 1999, 103, 11004-11010.	1.1	15
68	Solvated molecular dynamics of LiCN isomerization: All-atom argon solvent versus a generalized Langevin bath. Journal of Chemical Physics, 2016, 144, 024104.	1.2	15
69	Neural network approach to time-dependent dividing surfaces in classical reaction dynamics. Physical Review E, 2018, 97, 042309.	0.8	15
70	An idealized model for nonequilibrium dynamics in molecular systems. Journal of Chemical Physics, 2005, 123, 144109.	1.2	14
71	The role of the CN vibration in the activated dynamics of LiNC$ightleftharpoons$â‡ŒLiCN isomerization in an argon solvent at high temperatures. Journal of Chemical Physics, 2014, 141, 074312.	1.2	14
72	Quantum and quasi-classical collisional dynamics of O₂â€“Ar at high temperatures. Journal of Chemical Physics, 2016, 144, 234311.	1.2	14

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73	Autonomous Computing Materials. ACS Nano, 2021, 15, 3586-3592.	7.3	14
74	Research highlights: examining the effect of shape on nanoparticle interactions with organisms. Environmental Science: Nano, 2016, 3, 696-700.	2.2	13
75	Influence of external driving on decays in the geometry of the LiCN isomerization. Journal of Chemical Physics, 2020, 153, 084115.	1.2	13
76	Energetics and structure of alanine-rich Î±-helices via adaptive steered molecular dynamics. Biophysical Journal, 2021, 120, 2009-2018.	0.2	13
77	Limits on the transition to Gaussian orthogonal ensemble behavior: Saturated radiationless transitions between strongly coupled potential surfaces. Physical Review A, 1989, 40, 5935-5949.	1.0	12
78	Dissipating the Langevin equation in the presence of an external stochastic potential. Journal of Chemical Physics, 2005, 122, 114111.	1.2	12
79	Dynamical simulation of dipolar Janus colloids: Dynamical properties. Journal of Chemical Physics, 2013, 138, 184903.	1.2	12
80	Unconventional aliphatic fluorophores discovered as the luminescence origin in citric acidâ€“urea carbon dots. Nanoscale, 2022, 14, 9516-9525.	2.8	12
81	Folding behavior of model proteins with weak energetic frustration. Journal of Chemical Physics, 2004, 120, 11292-11303.	1.2	11
82	Advancing The Chemical Sciences Through Diversity. Chemical & Engineering News, 2014, 92, 45.	0.2	11
83	Molecular dynamics out of equilibrium: mechanics and measurables. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 541-561.	6.2	11
84	Structure of a tractable stochastic mimic of soft particles. Soft Matter, 2014, 10, 5350-5361.	1.2	11
85	The Gender and URM Faculty Demographics Data Collected by OXIDE. ACS Symposium Series, 2017, , 101-112.	0.5	11
86	Mutational Analysis of Neuropeptide Y Reveals Unusual Thermal Stability Linked to Higher-Order Self-Association. ACS Omega, 2018, 3, 2141-2154.	1.6	11
87	Defects in Self-Assembled Monolayers on Nanoparticles Prompt Phospholipid Extraction and Bilayer-Curvature-Dependent Deformations. Journal of Physical Chemistry C, 2019, 123, 27951-27958.	1.5	11
88	Phase-space resolved rates in driven multidimensional chemical reactions. Journal of Chemical Physics, 2019, 151, 244108.	1.2	11
89	The relative stability of trpzip1 and its mutants determined by computation and experiment. RSC Advances, 2020, 10, 6520-6535.	1.7	11
90	Learning from the Machine: Uncovering Sustainable Nanoparticle Design Rules. Journal of Physical Chemistry C, 2020, 124, 13409-13420.	1.5	11

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91	A Phenomenological Model for Surface Diffusion:Â Diffusive Dynamics across Incoherent Stochastic Aperiodic Potentials. Journal of Physical Chemistry B, 2004, 108, 19476-19482.	1.2	10
92	Momentum and Velocity Autocorrelation Functions of a Diatomic Molecule Are Not Necessarily Proportional to Each Other. Journal of Physical Chemistry B, 2008, 112, 213-218.	1.2	10
93	Effects of Solute Structure on Local Solvation and Solvent Interactions: Results from UV/Vis Spectroscopy and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2008, 112, 14993-14998.	1.2	10
94	Surface Coating Structure and Its Interaction with Cytochrome c in EG₆-Coated Nanoparticles Varies with Surface Curvature. Langmuir, 2020, 36, 5030-5039.	1.6	10
95	Molecular Dynamics Simulations of Solvation and Solvent Reorganization Dynamics in CO₂-Expanded Methanol and Acetone. Journal of Chemical Theory and Computation, 2009, 5, 267-275.	2.3	9
96	Absence of Enhanced Diffusion in the Dynamics of a Thick Needle through Three-Dimensional Fixed Spherical Scatterers. Journal of Physical Chemistry B, 2011, 115, 4412-4418.	1.2	9
97	Diffusion of a Spherical Probe through Static Nematogens: Effect of Increasing Geometric Anisotropy and Long-Range Structure. Journal of Physical Chemistry B, 2012, 116, 1328-1334.	1.2	9
98	Stochastic dynamics of penetrable rods in one dimension: Occupied volume and spatial order. Journal of Chemical Physics, 2013, 138, 244901.	1.2	9
99	A Top-Down Approach for Diversity and Inclusion in Chemistry Departments. ACS Symposium Series, 2014, , 207-224.	0.5	9
100	Transition state theory for solvated reactions beyond recrossing-free dividing surfaces. Physical Review E, 2016, 93, 062304.	0.8	9
101	Ionic Environment Affects Bacterial Lipopolysaccharide Packing and Function. Langmuir, 2020, 36, 3149-3158.	1.6	9
102	Activated Dynamics Across Aperiodic Stochastic Potentialsâ€. Journal of Physical Chemistry B, 2002, 106, 8176-8181.	1.2	8
103	Revisiting roaming trajectories in ketene isomerization at higher dimensionality. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	8
104	Neural network approach for the dynamics on the normally hyperbolic invariant manifold of periodically driven systems. Physical Review E, 2020, 101, 022219.	0.8	8
105	On the stability of satellites at unstable libration points of sunâ€“planetâ€“moon systems. Communications in Nonlinear Science and Numerical Simulation, 2022, 104, 106053.	1.7	8
106	National Diversity Equity Workshop 2017: Focus on Underrepresented Minorities in Chemistry Faculties. ACS Symposium Series, 2018, , 109-140.	0.5	8
107	Electric Potential of Citrate-Capped Gold Nanoparticles Is Affected by Poly(allylamine hydrochloride) and Salt Concentration. ACS Applied Materials & Interfaces, 2022, 14, 12538-12550.	4.0	8
108	Implementation of Telescoping Boxes in Adaptive Steered Molecular Dynamics. Journal of Chemical Theory and Computation, 2022, 18, 4649-4659.	2.3	8

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109	An optimized mean first passage time approach for obtaining rates in activated processes. Journal of Chemical Physics, 2002, 117, 9227-9233.	1.2	7
110	National Diversity Equity Workshop 2013: Focus on Gender Identity and Orientation in Chemistry Faculties. ACS Symposium Series, 2018, , 51-77.	0.5	7
111	National Diversity Equity Workshop 2015: Intersectionality in Chemistry Faculties. ACS Symposium Series, 2018, , 79-107.	0.5	7
112	A two-dimensional polymer growth model. Journal of Chemical Physics, 2001, 115, 1575-1585.	1.2	6
113	A three-dimensional polymer growth model. Journal of Chemical Physics, 2002, 116, 10485-10491.	1.2	6
114	Dynamical simulation of electrostatic striped colloidal particles. Journal of Chemical Physics, 2014, 140, 034701.	1.2	6
115	Modeling soft core-shell colloids using stochastic hard collision dynamics. Chemical Physics Letters, 2018, 708, 233-240.	1.2	6
116	National Diversity Equity Workshop 2011: Lowering Barriers for all Underrepresented Chemistry Professors. ACS Symposium Series, 2018, , 21-49.	0.5	6
117	National Diversity Equity Workshops: Advancing Diversity in Academia. ACS Symposium Series, 2018, , 1-19.	0.5	6
118	Identifying reaction pathways in phase space via asymptotic trajectories. Physical Chemistry Chemical Physics, 2020, 22, 10087-10105.	1.3	6
119	Phase space geometry of isolated to condensed chemical reactions. Journal of Chemical Physics, 2021, 155, 210901.	1.2	6
120	Fast Numerical Integrator for Stochastic Differential Equations with Nonstationary Multiplicative Noiseâ€. Journal of Physical Chemistry A, 2001, 105, 2687-2693.	1.1	5
121	Nonequilibrium heat flows through a nanorod sliding across a surface. Journal of Chemical Physics, 2011, 134, 104703.	1.2	5
122	Temperature-driven irreversible generalized Langevin equation can capture the nonequilibrium dynamics of two dissipated coupled oscillators. Physical Review E, 2013, 88, 032145.	0.8	5
123	Effective Surface Coverage of Coarse-Grained Soft Matter. Journal of Physical Chemistry B, 2014, 118, 14092-14102.	1.2	5
124	Diversity In Academia: Solutions To Get There. Chemical & Engineering News, 2015, 93, 40.	0.2	5
125	Stochastic dynamics of penetrable rods in one dimension: Entangled dynamics and transport properties. Journal of Chemical Physics, 2015, 142, 154906.	1.2	5
126	Engineered nanoparticle network models for autonomous computing. Journal of Chemical Physics, 2021, 154, 214702.	1.2	5

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127	Dihedral-Angle Information Entropy as a Gauge of Secondary Structure Propensity. Biophysical Journal, 2006, 91, 4014-4023.	0.2	4
128	OneChemistry in the marketplace of ideas. C&EN Global Enterprise, 2017, 95, 41-41.	0.0	4
129	Variational principle for the determination of unstable periodic orbits and instanton trajectories at saddle points. Physical Review A, 2017, 95, .	1.0	4
130	Dynamics and decay rates of a time-dependent two-saddle system. Physical Review E, 2021, 103, 022121.	0.8	4
131	A Cuban Campesino in Chemistryâ€™s Academic Court. Journal of Physical Chemistry A, 2021, 125, 6505-6511.	1.1	4
132	Controlling reaction dynamics in chemical model systems through external driving. Physica D: Nonlinear Phenomena, 2021, 427, 133013.	1.3	4
133	Building blocks for autonomous computing materials: Dimers, trimers, and tetramers. Journal of Chemical Physics, 2021, 155, 154704.	1.2	4
134	Diffusion in a nonequilibrium binary mixture of hard spheres swelling at different rates. Journal of Chemical Physics, 2009, 131, 024503.	1.2	3
135	The Private Sectorâ€™s Role In Chemistryâ€™s Future. Chemical & Engineering News, 2015, 93, 33.	0.2	3
136	Dynamics and Bifurcations on the Normally Hyperbolic Invariant Manifold of a Periodically Driven System with Rank-1 Saddle. Regular and Chaotic Dynamics, 2020, 25, 496-507.	0.3	3
137	Optimizing bags of artificial neural networks for the prediction of viability from sparse data. Journal of Chemical Physics, 2020, 153, 054112.	1.2	3
138	Solvent softness effects on unimolecular chemical reaction rate constants. Chemical Physics Letters, 2020, 744, 137182.	1.2	3
139	Nonequilibrium structure in sequential assembly. Physical Review E, 2015, 92, 052108.	0.8	2
140	Kinetics of intra- and intermolecular excited-state proton transfer ofÏ‰-(2-hydroxynaphthyl-1)-decanoic acid in homogeneous and micellar solutions. Methods and Applications in Fluorescence, 2016, 4, 014001.	1.1	2
141	Accelerating Change: #DiversitySolutions on Social Media. ACS Symposium Series, 2017, , 67-75.	0.5	2
142	Nonstationary Stochastic Dynamics and Applications to Chemical Physics. Progress in Theoretical Chemistry and Physics, 2002, , 91-116.	0.2	2
143	Removing Barriers. ACS Symposium Series, 2020, , 91-108.	0.5	2
144	Molecular Structure of Single-Stranded DNA on the ZnS Surface of Quantum Dots. ACS Nano, 2022, 16, 6666-6675.	7.3	2

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145	Stochastic Models for Polymerization Reactions Under Nonequilibrium Conditions. Annual Reports in Computational Chemistry, 2008, 4, 173-199.	0.9	1
146	De novo identification of binding sequences for antibody replacement molecules. Proteins: Structure, Function and Bioinformatics, 2009, 76, 693-705.	1.5	1
147	Adaptive Steered Molecular Dynamics: Unfolding of Neuropeptide Y and Decaalanine Stretching. Biophysical Journal, 2011, 100, 524a.	0.2	1
148	Quantal treatment of O2–Ar vibrational relaxation at hypersonic temperatures. , 2017, , .		1
149	Thermal decay rates of an activated complex in a driven model chemical reaction. Physical Review E, 2020, 102, 062204.	0.8	1
150	A Cuban Campesino in Chemistryâ€™s Academic Court. Journal of Physical Chemistry C, 2021, 125, 16371-16377.	1.5	1
151	A Cuban Campesino in Chemistryâ€™s Academic Court. Journal of Physical Chemistry B, 2021, 125, 8261-8267.	1.2	1
152	Transition state dynamics of a driven magnetic free layer. Communications in Nonlinear Science and Numerical Simulation, 2022, 105, 106054.	1.7	1
153	Mean first-passage times for solvated LiCN isomerization at intermediate to high temperatures. Journal of Chemical Physics, 2022, 156, 034103.	1.2	1
154	Chapter 8 The Role of Long-Time Correlation in Dissipative Adsorbate Dynamics on Metal Surfaces. Annual Reports in Computational Chemistry, 2007, 3, 137-151.	0.9	0
155	Viewing the Cybotactic Structure of Gas-Expanded Liquids. ACS Symposium Series, 2009, , 81-94.	0.5	0
156	Sifting a Massive Virtual Library of Peptide Ligands for an Optimal Binder to a Given Receptor. Biophysical Journal, 2011, 100, 214a.	0.2	0
157	Academic leadership skills 101. C&EN Global Enterprise, 2016, 94, 47-47.	0.0	0
158	Leadership Training for Teacher-Scholars. ACS Symposium Series, 2017, , 35-49.	0.5	0
159	ACS: Your brick-and-mortar and virtual network all in one. C&EN Global Enterprise, 2018, 96, 34-34.	0.0	0
160	Order parameters in the diffusion of rods through two- and three-dimensional fixed scatterers. Physical Review E, 2018, 98, .	0.8	0
161	Surface Curvature and Aminated Side-Chain Partitioning Affect Structure of Poly(oxonorbornenes) Attached to Planar Surfaces and Nanoparticles of Gold. Langmuir, 2020, 36, 10412-10420.	1.6	0
162	Solvation Dynamics in the Cybotactic Region of Gas-Expanded Liquids: A Decade Later. Industrial & Engineering Chemistry Research, 2020, 59, 1646-1655.	1.8	0