George L Barnes

List of Publications by Year
in descending order

36 papers	1,054 citations	394421 19 h-index	414414 32 g-index
46 all docs	46 docs citations	46 times ranked	892 citing authors

#	Article	IF	Citations
1	<scp>AutoMeKin2021</scp>: An openâ€source program for automated reaction discovery. Journal of Computational Chemistry, 2021, 42, 2036-2048.	3.3	42
2	Exploring the Effects of Methylation on the CID of Protonated Lysine: A Combined Experimental and Computational Approach. Journal of the American Society for Mass Spectrometry, 2021, 32, 2675-2684.	2.8	2
3	Modeling the Effects of O-Sulfonation on the CID of Serine. Journal of the American Society for Mass Spectrometry, 2020, 31, 1114-1122.	2.8	8
4	Fast fragmentation during surface-induced dissociation: An examination of peptide size and structure. Chemical Physics Letters, 2020, 754, 137716.	2.6	6
5	Memorial Viewpoint for William L. Hase. Journal of Physical Chemistry A, 2020, 124, 4183-4184.	2.5	0
6	Role of Chemical Dynamics Simulations in Mass Spectrometry Studies of Collision-Induced Dissociation and Collisions of Biological Ions with Organic Surfaces. Journal of the American Society for Mass Spectrometry, 2020, 31, 2-24.	2.8	30
7	tsscds2018: A code for automated discovery of chemical reaction mechanisms and solving the kinetics. Journal of Computational Chemistry, 2018, 39, 1922-1930.	3.3	56
8	A Computational Comparison of Soft Landing of Î±-Helical vs Globular Peptides. Journal of Physical Chemistry B, 2018, 122, 9549-9554.	2.6	7
9	Direct Chemical Dynamics Simulations. Journal of the American Chemical Society, 2017, 139, 3570-3590.	13.7	128
10	Simulating the Effect of Charge State on Reactive Landing of a Cyclic Tetrapeptide on Chemically Modified Alkylthiolate Self-Assembled Monolayer Surfaces. Journal of Physical Chemistry C, 2017, 121, 14628-14635.	3.1	9
11	Model Simulations of the Thermal Dissociation of the TIK(H+)2 Tripeptide: Mechanisms and Kinetic Parameters. Journal of Physical Chemistry A, 2016, 120, 8211-8227.	2.5	34
12	Dynamics of Protonated Peptide Ion Collisions with Organic Surfaces: Consonance of Simulation and Experiment. Journal of Physical Chemistry Letters, 2016, 7, 3142-3150.	4.6	30
13	Chemical dynamics simulations of energy transfer, surface-induced dissociation, soft-landing, and reactive-landing in collisions of protonated peptide ions with organic surfaces. Chemical Society Reviews, 2016, 45, 3595-3608.	38.1	28
14	The effect of protonation site and conformation on surface-induced dissociation in a small, lysine containing peptide. Chemical Physics Letters, 2015, 637, 83-87.	2.6	11
15	Energy and temperature dependent dissociation of the Na+(benzene)1,2 clusters: Importance of anharmonicity. Journal of Chemical Physics, 2015, 142, 044306.	3.0	24
16	The Role of Proton Transfer in Surface-Induced Dissociation. Journal of Physical Chemistry C, 2014, 118, 22149-22155.	3.1	20
17	The VENUS/NWChem software package. Tight coupling between chemical dynamics simulations and electronic structure theory. Computer Physics Communications, 2014, 185, 1074-1080.	7.5	93
18	Complex Formation during SID and Its Effect on Proton Mobility. Journal of Physical Chemistry Letters, 2013, 4, 3935-3939.	4.6	21

#	Article	IF	Citations
19	Surface Deposition Resulting from Collisions between Diglycine and Chemically Modified Alkylthiolate Self-Assembled Monolayer Surfaces. Journal of Physical Chemistry C, 2013, 117, 13087-13093.	3.1	16
20	Time dependent quantum thermodynamics of a coupled quantum oscillator system in a small thermal environment. Journal of Chemical Physics, 2013, 139, 214108.	3.0	6
21	Visualizing the zero order basis of the spectroscopic Hamiltonian. Journal of Chemical Physics, 2012, 136, 024114.	3.0	3
22	Effective Hamiltonian for femtosecond vibrational dynamics. Journal of Chemical Physics, 2011, 135, 144113.	3.0	4
23	Fragmentation and reactivity in collisions of protonated diglycine with chemically modified perfluorinated alkylthiolate-self-assembled monolayer surfaces. Journal of Chemical Physics, 2011, 134, 094106.	3.0	37
24	Detailed analysis of polyad-breaking spectroscopic Hamiltonians for multiple minima with above barrier motion: Isomerization in HO2. Journal of Chemical Physics, 2011, 134, 074108.	3.0	14
25	Communication: Effective spectroscopic Hamiltonian for multiple minima with above barrier motion: Isomerization in HO2. Journal of Chemical Physics, 2010, 133, 101105.	3.0	11
26	Model non-equilibrium molecular dynamics simulations of heat transfer from a hot gold surface to an alkylthiolate self-assembled monolayer. Physical Chemistry Chemical Physics, 2010, 12, 4435.	2.8	18
27	Bent out of shape. Nature Chemistry, 2009, 1, 103-104.	13.6	17
28	NH₄⁺ + CH₄ Gas Phase Collisions as a Possible Analogue to Protonated Peptide/Surface Induced Dissociation. Journal of Physical Chemistry A, 2009, 113, 7543-7547.	2.5	6
29	Energy Transfer, Unfolding, and Fragmentation Dynamics in Collisions of N-Protonated Octaglycine with an H-SAM Surface. Journal of the American Chemical Society, 2009, 131, 17185-17193.	13.7	49
30	An equilibrium focused approach to calculating the Raman spectrum of the symmetric OH stretch in formic acid dimer. Journal of Molecular Spectroscopy, 2008, 249, 78-85.	1.2	26
31	Elucidating energy disposal pathways following excitation of the symmetric OH stretching band in formic acid dimer. Chemical Physics Letters, 2008, 460, 42-45.	2.6	9
32	Symmetric Double Proton Tunneling in Formic Acid Dimer:â€‰ A Diabatic Basis Approach. Journal of Physical Chemistry B, 2008, 112, 595-603.	2.6	53
33	The effects of asymmetric motions on the tunneling splittings in formic acid dimer. Journal of Chemical Physics, 2008, 129, 164317.	3.0	31
34	Ion imaging studies of product rotational alignment in collisions of NO with Ar. Chemical Physics, 2004, 301, 261-272.	1.9	47
35	Recombination and Reaction Dynamics Following Photodissociation of CH3OCl in Solution. Journal of Physical Chemistry A, 2004, 108, 10973-10979.	2.5	25
36	Direct Measurement of the Preferred Sense of NO Rotation After Collision with Argon. Science, 2001, 293, 2063-2066.	12.6	132