

George L Barnes

List of Publications by Year in descending order

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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	Direct Measurement of the Preferred Sense of NO Rotation After Collision with Argon. <i>Science</i> , 2001, 293, 2063-2066.	12.6	132
2	Direct Chemical Dynamics Simulations. <i>Journal of the American Chemical Society</i> , 2017, 139, 3570-3590.	13.7	128
3	The VENUS/NWChem software package. Tight coupling between chemical dynamics simulations and electronic structure theory. <i>Computer Physics Communications</i> , 2014, 185, 1074-1080.	7.5	93
4	tsscads2018: A code for automated discovery of chemical reaction mechanisms and solving the kinetics. <i>Journal of Computational Chemistry</i> , 2018, 39, 1922-1930.	3.3	56
5	Symmetric Double Proton Tunneling in Formic Acid Dimer: A Diabatic Basis Approach. <i>Journal of Physical Chemistry B</i> , 2008, 112, 595-603.	2.6	53
6	Energy Transfer, Unfolding, and Fragmentation Dynamics in Collisions of N-Protonated Octaglycine with an H-SAM Surface. <i>Journal of the American Chemical Society</i> , 2009, 131, 17185-17193.	13.7	49
7	Ion imaging studies of product rotational alignment in collisions of NO with Ar. <i>Chemical Physics</i> , 2004, 301, 261-272.	1.9	47
8	<sc>AutoMeKin2021</sc>: An open-source program for automated reaction discovery. <i>Journal of Computational Chemistry</i> , 2021, 42, 2036-2048.	3.3	42
9	Fragmentation and reactivity in collisions of protonated diglycine with chemically modified perfluorinated alkythiolate-self-assembled monolayer surfaces. <i>Journal of Chemical Physics</i> , 2011, 134, 094106.	3.0	37
10	Model Simulations of the Thermal Dissociation of the TIK(H ⁺) ₂ Tripeptide: Mechanisms and Kinetic Parameters. <i>Journal of Physical Chemistry A</i> , 2016, 120, 8211-8227.	2.5	34
11	The effects of asymmetric motions on the tunneling splittings in formic acid dimer. <i>Journal of Chemical Physics</i> , 2008, 129, 164317.	3.0	31
12	Dynamics of Protonated Peptide Ion Collisions with Organic Surfaces: Consonance of Simulation and Experiment. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3142-3150.	4.6	30
13	Role of Chemical Dynamics Simulations in Mass Spectrometry Studies of Collision-Induced Dissociation and Collisions of Biological Ions with Organic Surfaces. <i>Journal of the American Society for Mass Spectrometry</i> , 2020, 31, 2-24.	2.8	30
14	Chemical dynamics simulations of energy transfer, surface-induced dissociation, soft-landing, and reactive-landing in collisions of protonated peptide ions with organic surfaces. <i>Chemical Society Reviews</i> , 2016, 45, 3595-3608.	38.1	28
15	An equilibrium focused approach to calculating the Raman spectrum of the symmetric OH stretch in formic acid dimer. <i>Journal of Molecular Spectroscopy</i> , 2008, 249, 78-85.	1.2	26
16	Recombination and Reaction Dynamics Following Photodissociation of CH ₃ OCl in Solution. <i>Journal of Physical Chemistry A</i> , 2004, 108, 10973-10979.	2.5	25
17	Energy and temperature dependent dissociation of the Na ⁺ (benzene) _{1,2} clusters: Importance of anharmonicity. <i>Journal of Chemical Physics</i> , 2015, 142, 044306.	3.0	24
18	Complex Formation during SID and Its Effect on Proton Mobility. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 3935-3939.	4.6	21

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19	The Role of Proton Transfer in Surface-Induced Dissociation. <i>Journal of Physical Chemistry C</i> , 2014, 118, 22149-22155.	3.1	20
20	Model non-equilibrium molecular dynamics simulations of heat transfer from a hot gold surface to an alkylthiolate self-assembled monolayer. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 4435.	2.8	18
21	Bent out of shape. <i>Nature Chemistry</i> , 2009, 1, 103-104.	13.6	17
22	Surface Deposition Resulting from Collisions between Diglycine and Chemically Modified Alkylthiolate Self-Assembled Monolayer Surfaces. <i>Journal of Physical Chemistry C</i> , 2013, 117, 13087-13093.	3.1	16
23	Detailed analysis of polyad-breaking spectroscopic Hamiltonians for multiple minima with above barrier motion: Isomerization in HO ₂ . <i>Journal of Chemical Physics</i> , 2011, 134, 074108.	3.0	14
24	Communication: Effective spectroscopic Hamiltonian for multiple minima with above barrier motion: Isomerization in HO ₂ . <i>Journal of Chemical Physics</i> , 2010, 133, 101105.	3.0	11
25	The effect of protonation site and conformation on surface-induced dissociation in a small, lysine containing peptide. <i>Chemical Physics Letters</i> , 2015, 637, 83-87.	2.6	11
26	Elucidating energy disposal pathways following excitation of the symmetric OH stretching band in formic acid dimer. <i>Chemical Physics Letters</i> , 2008, 460, 42-45.	2.6	9
27	Simulating the Effect of Charge State on Reactive Landing of a Cyclic Tetrapeptide on Chemically Modified Alkylthiolate Self-Assembled Monolayer Surfaces. <i>Journal of Physical Chemistry C</i> , 2017, 121, 14628-14635.	3.1	9
28	Modeling the Effects of <i>O</i> -Sulfonation on the CID of Serine. <i>Journal of the American Society for Mass Spectrometry</i> , 2020, 31, 1114-1122.	2.8	8
29	A Computational Comparison of Soft Landing of α -Helical vs Globular Peptides. <i>Journal of Physical Chemistry B</i> , 2018, 122, 9549-9554.	2.6	7
30	NH ₄ ⁺ + CH ₄ Gas Phase Collisions as a Possible Analogue to Protonated Peptide/Surface Induced Dissociation. <i>Journal of Physical Chemistry A</i> , 2009, 113, 7543-7547.	2.5	6
31	Time dependent quantum thermodynamics of a coupled quantum oscillator system in a small thermal environment. <i>Journal of Chemical Physics</i> , 2013, 139, 214108.	3.0	6
32	Fast fragmentation during surface-induced dissociation: An examination of peptide size and structure. <i>Chemical Physics Letters</i> , 2020, 754, 137716.	2.6	6
33	Effective Hamiltonian for femtosecond vibrational dynamics. <i>Journal of Chemical Physics</i> , 2011, 135, 144113.	3.0	4
34	Visualizing the zero order basis of the spectroscopic Hamiltonian. <i>Journal of Chemical Physics</i> , 2012, 136, 024114.	3.0	3
35	Exploring the Effects of Methylation on the CID of Protonated Lysine: A Combined Experimental and Computational Approach. <i>Journal of the American Society for Mass Spectrometry</i> , 2021, 32, 2675-2684.	2.8	2
36	Memorial Viewpoint for William L. Hase. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4183-4184.	2.5	0