

Xinyou

List of Publications by Year in descending order

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23
papers

494
citations

759233

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h-index

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all docs

23
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23
times ranked

555
citing authors

#	ARTICLE	IF	CITATIONS
1	Structural Characterization of Protonated Water Clusters Confined in HZSM-5 Zeolites. <i>Journal of the American Chemical Society</i> , 2021, 143, 10203-10213.	13.7	35
2	Advanced Materials for Energy-Water Systems: The Central Role of Water/Solid Interfaces in Adsorption, Reactivity, and Transport. <i>Chemical Reviews</i> , 2021, 121, 9450-9501.	47.7	43
3	Single Solvent Molecules Induce Dual Nucleophiles in Gas-Phase Ion-Molecule Nucleophilic Substitution Reactions. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 7134-7139.	4.6	8
4	Differential Condensation of Methane Isotopologues Leading to Isotopic Enrichment under Non-equilibrium Gas-Surface Collision Conditions. <i>Journal of Physical Chemistry A</i> , 2021, 125, 9405-9413.	2.5	3
5	Water-Assisted Proton Transport in Confined Nanochannels. <i>Journal of Physical Chemistry C</i> , 2020, 124, 16186-16201.	3.1	12
6	Time-Dependent Perspective for the Intramolecular Couplings of the N-H Stretches of Protonated Tryptophan. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4062-4067.	2.5	1
7	Interaction between $\hat{I}^{3}C87$ and $\hat{I}^{3}R242$ residues participates in energy coupling between catalysis and proton translocation in <i>Escherichia coli</i> ATP synthase. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2019, 1860, 679-687.	1.0	5
8	Is CH ₃ NC isomerization an intrinsic non-RRKM unimolecular reaction?. <i>Journal of Chemical Physics</i> , 2019, 151, 184110.	3.0	4
9	Pronounced changes in atomistic mechanisms for the Cl ⁺ + CH ₃ I S _N 2 reaction with increasing collision energy. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 2039-2045.	2.8	5
10	Addressing an instability in unrestricted density functional theory direct dynamics simulations. <i>Journal of Computational Chemistry</i> , 2019, 40, 933-936.	3.3	3
11	PSO Method for Fitting Analytic Potential Energy Functions. Application to H ₂ O. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1321-1332.	5.3	5
12	Direct dynamics simulations of the unimolecular dissociation of dioxetane: Probing the non-RRKM dynamics. <i>Journal of Chemical Physics</i> , 2018, 148, 164309.	3.0	12
13	Model-Based Analyses of Confined Polymer Electrolyte Nanothin Films Experimentally Probed by Polarized ATR-FTIR Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2018, 122, 9578-9585.	3.1	13
14	Effects of vibrational and rotational energies on the lifetime of the pre-reaction complex for the F ⁺ + CH ₃ I S _N 2 reaction. <i>International Journal of Mass Spectrometry</i> , 2018, 429, 127-135.	1.5	11
15	A quantum mechanical insight into S _N 2 reactions: Semiclassical initial value representation calculations of vibrational features of the Cl ⁺ -CH ₃ Cl pre-reaction complex with the VENUS suite of codes. <i>Journal of Chemical Physics</i> , 2018, 149, 164113.	3.0	19
16	Anharmonic Densities of States for Vibrationally Excited I ⁺ (H ₂ O) ₂ , (H ₂ O) ₂ , and I ⁺ (H ₂ O) ₂ . <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3986-3997.	5.3	8
17	Competing E2 and S _N 2 Mechanisms for the F ⁺ + CH ₃ CH ₂ I Reaction. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1078-1085.	2.5	26
18	Effect of microsolvation on the OH ⁺ (H ₂ O) _n + CH ₃ I rate constant. comparison of experiment and calculations for OH ⁺ (H ₂ O) ₂ + CH ₃ I. <i>International Journal of Mass Spectrometry</i> , 2017, 418, 122-129.	1.5	20

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19	Direct Chemical Dynamics Simulations. Journal of the American Chemical Society, 2017, 139, 3570-3590.	13.7	128
20	Perspective: chemical dynamics simulations of non-statistical reaction dynamics. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2017, 375, 20160204.	3.4	63
21	Post-transition state dynamics and product energy partitioning following thermal excitation of the F ⁺ HCH ₂ CN transition state: Disagreement with experiment. Journal of Chemical Physics, 2017, 147, 144301.	3.0	14
22	Potential energy surface stationary points and dynamics of the F ⁺ +CH ₃ I double inversion mechanism. Physical Chemistry Chemical Physics, 2017, 19, 20127-20136.	2.8	31
23	Chemical Dynamics Simulations of Benzene Dimer Dissociation. Journal of Physical Chemistry A, 2015, 119, 6631-6640.	2.5	25