Jiaxu Zhang

List of Publications by Year
in descending order

38 papers	1,242 citations	361413 20 h-index	361022 35 g-index
38 all docs	38 docs citations	38 times ranked	583 citing authors

#	Article	IF	Citations
1	Phase-controllable polymerized ionic liquids for CO₂ fixation into cyclic carbonates. Sustainable Energy and Fuels, 2021, 5, 1026-1033.	4.9	23
2	Direct dynamics simulations on the atomic mechanisms of 4O+Â+ CH3I reaction. International Journal of Mass Spectrometry, 2021, 461, 116504.	1.5	0
3	Effect of water on dynamics of HOCO radical. Chemical Physics, 2021, 546, 111173.	1.9	0
4	Direct dynamics in a proton transfer reaction of isomer product competition. Insight into the suppressed formation of the isoformyl cation. Physical Chemistry Chemical Physics, 2021, 23, 10814-10821.	2.8	0
5	Facile fabrication of a heterogeneous Co-modified pyridinecarboxaldehyde-polyethylenimine catalyst for efficient CO₂ conversion under mild conditions. Inorganic Chemistry Frontiers, 2020, 7, 1140-1147.	6.0	8
6	Direct Dynamics Simulations of the Thermal Fragmentation of a Protonated Peptide Containing Arginine. ACS Omega, 2020, 5, 1463-1471.	3.5	5
7	Theoretical Study of the Potential Energy Profile of the HBr⁺ + CO₂ â†' HOCO⁺ + BrÂ· Reaction. Journal of Physical Chemistry A, 2019, 123, 9791-9799.	2.5	4
8	Energy Transfer of Peptide Ions Colliding with a Selfâ€Assembled Monolayer Surface. The Influence of Peptide Ion Size. Chinese Journal of Chemistry, 2019, 37, 237.	4.9	1
9	Dynamics of Cl^{â€"}(H₂O) + CH₃I Substitution Reaction: The Influences of Solvent and Nucleophile. Journal of Physical Chemistry A, 2019, 123, 2203-2210.	2.5	6
10	Carbon Dioxide Activation and Conversion by Hyperbranched Polyethylenimine/ZnI₂ Catalysts. Industrial & Engineering Chemistry Research, 2019, 58, 872-878.	3.7	7
11	Facile synthesis of DBU-based ionic liquids cooperated with ZnI 2 as catalysts for efficient cycloaddition of CO 2 to epoxides under mild and solvent-free conditions. Molecular Catalysis, 2018, 450, 39-45.	2.0	43
12	Competition of F/OH-Induced S_N2 and Proton-Transfer Reactions with Increased Solvation. Journal of Physical Chemistry A, 2018, 122, 9446-9453.	2.5	14
13	How a Solvent Molecule Affects Competing Elimination and Substitution Dynamics. Insight into Mechanism Evolution with Increased Solvation. Journal of the American Chemical Society, 2018, 140, 10995-11005.	13.7	46
14	Competing E2 and S_N2 Mechanisms for the F^{â€"} + CH₃CH₂I Reaction. Journal of Physical Chemistry A, 2017, 121, 1078-1085.	2.5	26
15	Effect of microsolvation on the OHâ^'(H2O)n+ CH3I rate constant. comparison of experiment and calculations for OHâ^'(H2O)2+ CH3I. International Journal of Mass Spectrometry, 2017, 418, 122-129.	1.5	20
16	Steric Effects of Solvent Molecules on S_N2 Substitution Dynamics. Journal of Physical Chemistry Letters, 2017, 8, 1885-1892.	4.6	31
17	Effects of Water Molecule on CO Oxidation by OH: Reaction Pathways, Kinetic Barriers, and Rate Constants. Journal of Physical Chemistry A, 2017, 121, 4868-4880.	2.5	10
18	Imaging dynamic fingerprints of competing E2 and SN2 reactions. Nature Communications, 2017, 8, 25.	12.8	59

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19	Effects of microsolvation on a S_N2 reaction: indirect atomistic dynamics and weakened suppression of reactivity. Physical Chemistry Chemical Physics, 2017, 19, 9992-9999.	2.8	21
20	Potential energy surface stationary points and dynamics of the F^{â˜'}+ CH₃I double inversion mechanism. Physical Chemistry Chemical Physics, 2017, 19, 20127-20136.	2.8	31
21	Indirect dynamics in S_N2@N: insight into the influence of central atoms. Physical Chemistry Chemical Physics, 2017, 19, 22691-22699.	2.8	12
22	Theoretical Studies on F^{â€“} + NH₂Cl Reaction: Nucleophilic Substitution at Neutral Nitrogen. Journal of Physical Chemistry A, 2016, 120, 3740-3746.	2.5	14
23	Electronic Structure Theory Study of the Microsolvated F^{â€“}(H₂O) + CH₃I S_N2 Reaction. Journal of Physical Chemistry A, 2016, 120, 3613-3622.	2.5	16
24	Microsolvated F^{â€“}(H₂O) + CH₃I S_N2 Reaction Dynamics. Insight into the Suppressed Formation of Solvated Products. Journal of Physical Chemistry Letters, 2016, 7, 660-665.	4.6	31
25	Theoretical study on the photodegradation reaction of deca-BDE in THF in the presence of furan. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	2
26	Comparison of direct dynamics simulations with different electronic structure methods. F^{â˜'} + CH₃I with MP2 and DFT/B97-1. Physical Chemistry Chemical Physics, 2015, 17, 2589-2597.	2.8	47
27	Dynamics of the F^{â€“} + CH₃I â†' HF + CH₂I^{â€“} Proton Transfer Reaction. Journal of Physical Chemistry A, 2015, 119, 12517-12525.	2.5	34
28	Is there hydrogen bonding for gas phase SN2 pre-reaction complexes?. International Journal of Mass Spectrometry, 2015, 378, 14-19.	1.5	34
29	The Fâ˜'+ CH3I â†' FCH3+ Iâ˜' entrance channel potential energy surface. International Journal of Mass Spectrometry, 2015, 377, 222-227.	1.5	19
30	Identification of Atomic-Level Mechanisms for Gas-Phase X^{â€“} + CH₃Y S_N2 Reactions by Combined Experiments and Simulations. Accounts of Chemical Research, 2014, 47, 2960-2969.	15.6	127
31	Indirect Dynamics in a Highly Exoergic Substitution Reaction. Journal of the American Chemical Society, 2013, 135, 4250-4259.	13.7	94
32	Simulation studies of the Clâ˜' + CH3I SN2 nucleophilic substitution reaction: Comparison with ion imaging experiments. Journal of Chemical Physics, 2013, 138, 114309.	3.0	55
33	Chemical Dynamics Simulations of the Hydroxyl Radical Reaction with Ethene. Chinese Journal of Chemical Physics, 2013, 26, 765-773.	1.3	7
34	Chemical Dynamics Simulations of X^{â€“} + CH₃Y â†' XCH₃ + Y^{â€“} Gas-Phase S_N2 Nucleophilic Substitution Reactions. Nonstatistical Dynamics and Nontraditional Reaction Mechanisms. Journal of Physical Chemistry A, 2012, 116, 3061-3080.	2.5	139
35	The Need for Enzymatic Steering in Abietic Acid Biosynthesis: Gas-Phase Chemical Dynamics Simulations of Carbocation Rearrangements on a Bifurcating Potential Energy Surface. Journal of the American Chemical Society, 2011, 133, 8335-8343.	13.7	69
36	Electronic Structure Theory Study of the F^{â˜'} + CH₃I â†' FCH₃ + I^{â˜'} Potential Energy Surface. Journal of Physical Chemistry A, 2010, 114, 9635-9643.	2.5	55

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37	F^{â˜'} + CH₃I â†' FCH₃ + I^{â˜'} Reaction Dynamics. Nontraditional Atomistic Mechanisms and Formation of a Hydrogen-Bonded Complex. Journal of Physical Chemistry Letters, 2010, 1, 2747-2752.	4.6	103
38	Quantum Chemical Calculations of the Cl^{â˜'} + CH₃I â†' CH₃Cl + I^{â˜'} Potential Energy Surface. Journal of Physical Chemistry A, 2009, 113, 1976-1984.	2.5	29