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	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
2	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
3	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
4	Indirect Dynamics in a Highly Exoergic Substitution Reaction. Journal of the American Chemical Society, 2013, 135, 4250-4259.	13.7	94
5	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
6	Imaging dynamic fingerprints of competing E2 and SN2 reactions. Nature Communications, 2017, 8, 25.	12.8	59
7	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
8	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
9	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
10	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
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	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
13	Is there hydrogen bonding for gas phase SN2 pre-reaction complexes?. International Journal of Mass Spectrometry, 2015, 378, 14-19.	1.5	34
14	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
15	Steric Effects of Solvent Molecules on S_N2 Substitution Dynamics. Journal of Physical Chemistry Letters, 2017, 8, 1885-1892.	4.6	31
16	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
17	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
18	Competing E2 and S_N2 Mechanisms for the F^{â€“} + CH₃CH₂I Reaction. Journal of Physical Chemistry A, 2017, 121, 1078-1085.	2.5	26

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19	Phase-controllable polymerized ionic liquids for CO₂ fixation into cyclic carbonates. Sustainable Energy and Fuels, 2021, 5, 1026-1033.	4.9	23
20	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
21	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
22	The Fâ¯+ CH3I â† FCH3+ Iâ¯ entrance channel potential energy surface. International Journal of Mass Spectrometry, 2015, 377, 222-227.	1.5	19
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	Theoretical Studies on F^{â€“} + NH₂Cl Reaction: Nucleophilic Substitution at Neutral Nitrogen. Journal of Physical Chemistry A, 2016, 120, 3740-3746.	2.5	14
25	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
26	Indirect dynamics in S_N2@N: insight into the influence of central atoms. Physical Chemistry Chemical Physics, 2017, 19, 22691-22699.	2.8	12
27	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
28	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
29	Chemical Dynamics Simulations of the Hydroxyl Radical Reaction with Ethene. Chinese Journal of Chemical Physics, 2013, 26, 765-773.	1.3	7
30	Carbon Dioxide Activation and Conversion by Hyperbranched Polyethylenimine/ZnI₂ Catalysts. Industrial & Engineering Chemistry Research, 2019, 58, 872-878.	3.7	7
31	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
32	Direct Dynamics Simulations of the Thermal Fragmentation of a Protonated Peptide Containing Arginine. ACS Omega, 2020, 5, 1463-1471.	3.5	5
33	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
34	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
35	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
36	Direct dynamics simulations on the atomic mechanisms of 4O+Â+ CH3I reaction. International Journal of Mass Spectrometry, 2021, 461, 116504.	1.5	0

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37	Effect of water on dynamics of HOCO radical. Chemical Physics, 2021, 546, 111173.	1.9	0
38	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