William Hase

List of Publications by Year
in descending order

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400 papers	18,756 citations	12303 69 h-index	27345 106 g-index
437 all docs	437 docs citations	437 times ranked	5436 citing authors

#	Article	IF	Citations
1	Direct dynamics simulation of the thermal O(³P)â€‰+â€‰dimethylamine reaction in the triplet surface. I. Rate constant and product branching. Journal of Physical Organic Chemistry, 2023, 36, .	0.9	3
2	Chemical dynamics simulations of energy transfer in CH₄ and N₂ collisions. RSC Advances, 2021, 11, 16173-16178.	1.7	0
3	Direct Dynamics Simulations of the ³CH₂ + ³O₂ Reaction at High Temperature. Journal of Physical Chemistry A, 2021, 125, 621-627.	1.1	1
4	Sampling initial positions and momenta for nuclear trajectories from quantum mechanical distributions. Journal of Chemical Physics, 2021, 154, 074115.	1.2	6
5	A chemical dynamics study of the HClÂ+ HCl+ reaction. International Journal of Mass Spectrometry, 2021, 462, 116515.	0.7	7
6	Direct Dynamics Simulations of Hyperthermal O(3P) Collisions with Pristine, Defected, Oxygenated, and Nitridated Graphene Surfaces. Journal of Physical Chemistry C, 2021, 125, 9795-9808.	1.5	10
7	Mechanism and kinetics for the reaction of methyl peroxy radical with O₂. Physical Chemistry Chemical Physics, 2021, 23, 23508-23516.	1.3	0
8	Unimolecular Fragmentation Properties of Thermometer Ions from Chemical Dynamics Simulations. Journal of the American Society for Mass Spectrometry, 2021, 32, 169-179.	1.2	5
9	Dynamics of Pyrene-Dimer Association and Ensuing Pyrene-Dimer Dissociation. Journal of Physical Chemistry A, 2020, 124, 8907-8917.	1.1	17
10	Collisional dynamics simulations revealing fragmentation properties of Zn(<scp>ii</scp>)-bound poly-peptide. Physical Chemistry Chemical Physics, 2020, 22, 14551-14559.	1.3	5
11	Exploring reactivity and product formation in N(4S) collisions with pristine and defected graphene with direct dynamics simulations. Journal of Chemical Physics, 2020, 153, 184702.	1.2	13
12	Comparison of intermolecular energy transfer from vibrationally excited benzene in mixed nitrogenâ€“benzene baths at 140 K and 300 K. Journal of Chemical Physics, 2020, 153, 144116.	1.2	6
13	Theoretical Study of the Dynamics of the HBr⁺ + CO₂ â†’ HOCO⁺ + Br Reaction. Journal of Physical Chemistry A, 2020, 124, 9119-9127.	1.1	10
14	Nonstatistical Reaction Dynamics. Annual Review of Physical Chemistry, 2020, 71, 289-313.	4.8	20
15	Comparison of Exponential and Biexponential Models of the Unimolecular Decomposition Probability for the Hinshelwoodâ€“Lindemann Mechanism. Journal of Physical Chemistry Letters, 2020, 11, 2772-2774.	2.1	0
16	Direct Dynamics Simulations of the Unimolecular Decomposition of the Randomly Excited ¹CH₂O₂ Criegee Intermediate. Comparison with ³CH₂ + ³O₂ Reaction Dynamics. Journal of Physical Chemistry A, 2020, 124, 1821-1828.	1.1	3
17	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.	1.2	30
18	Direct Dynamics Simulations of the Thermal Fragmentation of a Protonated Peptide Containing Arginine. ACS Omega, 2020, 5, 1463-1471.	1.6	5

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19	Time-Dependent Perspective for the Intramolecular Couplings of the Nâ€“H Stretches of Protonated Tryptophan. Journal of Physical Chemistry A, 2020, 124, 4062-4067.	1.1	1
20	Editorial: Application of Optimization Algorithms in Chemistry. Frontiers in Chemistry, 2020, 8, 198.	1.8	1
21	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	1.2	42
22	Direct Dynamics Simulations of Fragmentation of a Zn(II)-2Cys-2His Oligopeptide. Comparison with Mass Spectrometry Collision-Induced Dissociation. Journal of Physical Chemistry A, 2019, 123, 6868-6885.	1.1	9
23	Is CH3NC isomerization an intrinsic non-RRKM unimolecular reaction?. Journal of Chemical Physics, 2019, 151, 184110.	1.2	4
24	Potential Energy Curves for Formation of the CH2O2 Criegee Intermediate on the 3CH2 + 3O2 Singlet and Triplet Potential Energy Surfaces. Journal of Physical Chemistry A, 2019, 123, 8968-8975.	1.1	5
25	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.	2.6	1
26	Pronounced changes in atomistic mechanisms for the Cl^{â^’} + CH₃I S_N2 reaction with increasing collision energy. Physical Chemistry Chemical Physics, 2019, 21, 2039-2045.	1.3	5
27	Direct Dynamics Simulations of the CH2 + O2 Reaction on the Ground- and Excited-State Singlet Surfaces. Journal of Physical Chemistry A, 2019, 123, 4360-4369.	1.1	6
28	<scp>l</scp>-Cysteine Modified by S-Sulfation: Consequence on Fragmentation Processes Elucidated by Tandem Mass Spectrometry and Chemical Dynamics Simulations. Journal of Physical Chemistry A, 2019, 123, 3685-3696.	1.1	20
29	Unimolecular Rate Constants versus Energy and Pressure as a Convolution of Unimolecular Lifetime and Collisional Deactivation Probabilities. Analyses of Intrinsic Non-RRKM Dynamics. Journal of Physical Chemistry A, 2019, 123, 1923-1928.	1.1	7
30	Chemical Dynamics Simulation of Energy Transfer: Propylbenzene Cation and N₂ Collisions. Journal of Physical Chemistry A, 2019, 123, 2301-2309.	1.1	9
31	Dynamics of proton transfer from ArH+ to CO. International Journal of Mass Spectrometry, 2019, 438, 175-185.	0.7	5
32	Structures and binding energies for complexations of different spin states of Ni⁺ and Ni²⁺ to aromatic molecules. Molecular Physics, 2019, 117, 1392-1403.	0.8	4
33	Correlation between the velocity scattering angle and product relative translational energy for SN2 reactions. Comparison of experiments and direct dynamics simulations. International Journal of Mass Spectrometry, 2019, 438, 115-123.	0.7	5
34	Addressing an instability in unrestricted density functional theory direct dynamics simulations. Journal of Computational Chemistry, 2019, 40, 933-936.	1.5	3
35	Unimolecular Fragmentation of Deprotonated Diproline [Pro₂-H]^{â^’} Studied by Chemical Dynamics Simulations and IRMPD Spectroscopy. Journal of Physical Chemistry A, 2018, 122, 2612-2625.	1.1	18
36	Direct Dynamics Simulation of the Thermal 3CH2 + 3O2 Reaction. Rate Constant and Product Branching Ratios. Journal of Physical Chemistry A, 2018, 122, 4808-4818.	1.1	11

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37	Chemical dynamics simulations of CID of peptide ions: comparisons between TIK(H⁺)₂and TLK(H⁺)₂fragmentation dynamics, and with thermal simulations. Physical Chemistry Chemical Physics, 2018, 20, 3614-3629.	1.3	18
38	PSO Method for Fitting Analytic Potential Energy Functions. Application to Iâ€“(H2O). Journal of Chemical Theory and Computation, 2018, 14, 1321-1332.	2.3	5
39	Gas Phase Synthesis of Protonated Glycine by Chemical Dynamics Simulations. Journal of Physical Chemistry A, 2018, 122, 869-877.	1.1	19
40	Nascent energy distribution of the Criegee intermediate CH2OO from direct dynamics calculations of primary ozonide dissociation. Journal of Chemical Physics, 2018, 148, 174306.	1.2	36
41	Direct dynamics simulations of the unimolecular dissociation of dioxetane: Probing the non-RRKM dynamics. Journal of Chemical Physics, 2018, 148, 164309.	1.2	12
42	Chemical Dynamics Simulations of Thermal Desorption of Protonated Dialanine from a Perfluorinated Self-Assembled Monolayer Surface. Journal of Physical Chemistry Letters, 2018, 9, 1554-1560.	2.1	3
43	Effects of vibrational and rotational energies on the lifetime of the pre-reaction complex for the Fâ¯+ CH3I SN2 reaction. International Journal of Mass Spectrometry, 2018, 429, 127-135.	0.7	11
44	Chemical Dynamics Simulation of Low Energy N₂ Collisions with Graphite. Journal of Physical Chemistry C, 2018, 122, 612-623.	1.5	17
45	Non-statistical intermolecular energy transfer from vibrationally excited benzene in a mixed nitrogen-benzene bath. Journal of Chemical Physics, 2018, 149, 134101.	1.2	15
46	Exploratory Direct Dynamics Simulations of ³O₂ Reaction with Graphene at High Temperatures. Journal of Physical Chemistry C, 2018, 122, 29368-29379.	1.5	13
47	A quantum mechanical insight into SN2 reactions: Semiclassical initial value representation calculations of vibrational features of the Clâ¯â¯CH3Cl pre-reaction complex with the VENUS suite of codes. Journal of Chemical Physics, 2018, 149, 164113.	1.2	19
48	Anharmonic Densities of States for Vibrationally Excited I^{â€“}(H₂O), (H₂O)₂, and I^{â€“}(H₂O)₂. Journal of Chemical Theory and Computation, 2018, 14, 3986-3997.	2.3	8
49	Chemical Dynamics Simulations and Scattering Experiments for O₂ Collisions with Graphite. Journal of Physical Chemistry C, 2018, 122, 16048-16059.	1.5	19
50	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.	6.6	46
51	Threshold for shattering fragmentation in collision-induced dissociation of the doubly protonated tripeptide TIK(H⁺)₂. Physical Chemistry Chemical Physics, 2018, 20, 19744-19749.	1.3	13
52	Competing E2 and S_N2 Mechanisms for the F^{â€“} + CH₃CH₂I Reaction. Journal of Physical Chemistry A, 2017, 121, 1078-1085.	1.1	26
53	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.	0.7	20
54	Direct Chemical Dynamics Simulations. Journal of the American Chemical Society, 2017, 139, 3570-3590.	6.6	128

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55	Steric Effects of Solvent Molecules on S_N2 Substitution Dynamics. Journal of Physical Chemistry Letters, 2017, 8, 1885-1892.	2.1	31
56	Collisional Intermolecular Energy Transfer from a N₂ Bath at Room Temperature to a Vibrationlly â€œColdâ€•C₆F₆ Molecule Using Chemical Dynamics Simulations. Journal of Physical Chemistry A, 2017, 121, 4049-4057.	1.1	15
57	Imaging dynamic fingerprints of competing E2 and SN2 reactions. Nature Communications, 2017, 8, 25.	5.8	59
58	Theoretical and computational studies of non-equilibrium and non-statistical dynamics in the gas phase, in the condensed phase and at interfaces. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2017, 375, 20170035.	1.6	18
59	Perspective: chemical dynamics simulations of non-statistical reaction dynamics. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2017, 375, 20160204.	1.6	63
60	Post-transition state dynamics and product energy partitioning following thermal excitation of the Fâ‹¯HCH2CN transition state: Disagreement with experiment. Journal of Chemical Physics, 2017, 147, 144301.	1.2	14
61	Chemical Dynamics Simulations of Energy Transfer for Propylbenzene Cation and He Collisions. Journal of Physical Chemistry A, 2017, 121, 7494-7502.	1.1	14
62	Data Reduction Through Increased Data Utilization in Chemical Dynamics Simulations. Big Data Research, 2017, 9, 57-66.	2.6	1
63	Potential energy surface stationary points and dynamics of the F^{â^’}+ CH₃I double inversion mechanism. Physical Chemistry Chemical Physics, 2017, 19, 20127-20136.	1.3	31
64	Electronic nature of zwitterionic alkali metal methanides, silanides and germanides â€“ a combined experimental and computational approach. Chemical Science, 2017, 8, 1316-1328.	3.7	23
65	Rethinking the S _N 2 reaction. Science, 2016, 352, 32-33.	6.0	146
66	Unimolecular dissociation of peptides: statistical vs. non-statistical fragmentation mechanisms and time scales. Faraday Discussions, 2016, 195, 599-618.	1.6	27
67	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.	1.1	34
68	Dynamics of Protonated Peptide Ion Collisions with Organic Surfaces: Consonance of Simulation and Experiment. Journal of Physical Chemistry Letters, 2016, 7, 3142-3150.	2.1	30
69	SYNTHESIS OF FORMAMIDE AND RELATED ORGANIC SPECIES IN THE INTERSTELLAR MEDIUM VIA CHEMICAL DYNAMICS SIMULATIONS. Astrophysical Journal, 2016, 826, 107.	1.6	24
70	Chemical Dynamics Simulations of Intermolecular Energy Transfer: Azulene + N₂ Collisions. Journal of Physical Chemistry A, 2016, 120, 5187-5196.	1.1	20
71	Zero-Point Energy Constraint for Unimolecular Dissociation Reactions. Giving Trajectories Multiple Chances To Dissociate Correctly. Journal of Physical Chemistry A, 2016, 120, 372-378.	1.1	29
72	Post-Transition State Dynamics in Gas Phase Reactivity: Importance of Bifurcations and Rotational Activation. Journal of Chemical Theory and Computation, 2016, 12, 974-982.	2.3	22

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73	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.	2.1	31
74	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.	18.7	28
75	Determination of the Temperature-Dependent OH^{â˜}â€‰(H₂O)â€¯+â€¯CH₃I Rate Constant by Experiment and Simulation. Zeitschrift Fur Physikalische Chemie, 2015, 229, 1747-1763.	1.4	21
76	Chemical dynamics simulations of the monohydrated OHâ˜(H2O) + CH3I reaction. Atomic-level mechanisms and comparison with experiment. Journal of Chemical Physics, 2015, 142, 244308.	1.2	53
77	Direct Dynamics Simulation of Dissociation of the [CH₃--I--OH]^{â˜} Ionâ€“Molecule Complex. Journal of Physical Chemistry A, 2015, 119, 817-825.	1.1	16
78	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.	1.3	47
79	Mechanistic details of energy transfer and soft landing in ala₂-H⁺ collisions with a F-SAM surface. Physical Chemistry Chemical Physics, 2015, 17, 24576-24586.	1.3	8
80	Bath Model for N₂ + C₆F₆ Gas-Phase Collisions. Details of the Intermolecular Energy Transfer Dynamics. Journal of Physical Chemistry C, 2015, 119, 14683-14691.	1.5	22
81	Dynamics of Na+(Benzene) + Benzene Association and Ensuing Na+(Benzene)2* Dissociation. Journal of Physical Chemistry A, 2015, 119, 7894-7904.	1.1	15
82	Chemical Dynamics Simulations of Benzene Dimer Dissociation. Journal of Physical Chemistry A, 2015, 119, 6631-6640.	1.1	25
83	Potential energy surfaces for the HBr+ + CO2 â†’ Br + HOCO+ reaction in the HBr+â€‰2Î3/2 and 2Î1/2 spin-orbit states. Journal of Chemical Physics, 2015, 142, 104302.	1.2	6
84	Energy and temperature dependent dissociation of the Na+(benzene)1,2 clusters: Importance of anharmonicity. Journal of Chemical Physics, 2015, 142, 044306.	1.2	24
85	Dynamics of the F^{â€“} + CH₃I â†’ HF + CH₂I^{â€“} Proton Transfer Reaction. Journal of Physical Chemistry A, 2015, 119, 12517-12525.	1.1	34
86	Is there hydrogen bonding for gas phase SN2 pre-reaction complexes?. International Journal of Mass Spectrometry, 2015, 378, 14-19.	0.7	34
87	The Fâ˜+ CH3I â†’ FCH3+ Iâ˜ entrance channel potential energy surface. International Journal of Mass Spectrometry, 2015, 377, 222-227.	0.7	19
88	A unified model for simulating liquid and gas phase, intermolecular energy transfer: N2 + C6F6 collisions. Journal of Chemical Physics, 2014, 140, 194103.	1.2	30
89	Dynamics of energy transfer and soft-landing in collisions of protonated dialanine with perfluorinated self-assembled monolayer surfaces. Physical Chemistry Chemical Physics, 2014, 16, 23769-23778.	1.3	13
90	Understanding Energy Transfer in Gasâ€“Surface Collisions from Gas-Phase Models. Journal of Physical Chemistry C, 2014, 118, 2609-2621.	1.5	11

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91	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.	7.6	127
92	Unraveling the Factors That Control Soft Landing of Small Silyl Ions on Fluorinated Self-Assembled Monolayers. Journal of Physical Chemistry C, 2014, 118, 10159-10169.	1.5	5
93	The VENUS/NWChem software package. Tight coupling between chemical dynamics simulations and electronic structure theory. Computer Physics Communications, 2014, 185, 1074-1080.	3.0	93
94	Properties of Complexes Formed by Na⁺, Mg²⁺, and Fe²⁺ Binding with Benzene Molecules. Journal of Physical Chemistry A, 2014, 118, 9500-9511.	1.1	48
95	Intermolecular Potential for Binding of Protonated Peptide Ions with Perfluorinated Hydrocarbon Surfaces. Journal of Physical Chemistry B, 2014, 118, 5577-5588.	1.2	17
96	Direct Dynamics Simulation of the Activation and Dissociation of 1,5-Dinitrobiuret (HDNB). Journal of Physical Chemistry A, 2014, 118, 2228-2236.	1.1	12
97	A Zwitterionic Carbanion Frustrated by Boranes â€“ Dihydrogen Cleavage with Weak Lewis Acids via an â€œInverseâ€•Frustrated Lewis Pair Approach. Journal of the American Chemical Society, 2013, 135, 16066-16069.	6.6	69
98	Ab Initio Modeling of Excitonic and Charge-Transfer States in Organic Semiconductors: The PTB1/PCBM Low Band Gap System. Journal of the American Chemical Society, 2013, 135, 18252-18255.	6.6	59
99	Models for Intrinsic Non-RRKM Dynamics. Decomposition of the SN2 Intermediate Clâ€“â€“CH3Br. Zeitschrift Fur Physikalische Chemie, 2013, 227, .	1.4	8
100	Comparison of Cluster, Slab, and Analytic Potential Models for the Dimethyl Methylphosphonate (DMMP)/TiO₂(110) Intermolecular Interaction. Journal of Physical Chemistry C, 2013, 117, 17613-17622.	1.5	18
101	Chemical Dynamics Simulations of High Energy Xenon Atom Collisions with the {0001} Surface of Hexagonal Ice. Journal of Physical Chemistry C, 2013, 117, 2183-2193.	1.5	11
102	A Load-Balancing Force Decomposition Scheme for Parallel Simulation of Chemical Dynamics with Multiple Inter-atomic Force Models. , 2013, , .		0
103	Direct Dynamics Simulations of the Product Channels and Atomistic Mechanisms for the OH^{â€“} + CH₃I Reaction. Comparison with Experiment. Journal of Physical Chemistry A, 2013, 117, 7162-7178.	1.1	73
104	Direct chemical dynamics simulations: coupling of classical and quasiclassical trajectories with electronic structure theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 296-316.	6.2	93
105	Evaluating the Accuracy of Hessian Approximations for Direct Dynamics Simulations. Journal of Chemical Theory and Computation, 2013, 9, 54-64.	2.3	44
106	Temperature Dependence of the OH^{â€“} + CH₃I Reaction Kinetics. Experimental and Simulation Studies and Atomic-Level Dynamics. Journal of Physical Chemistry A, 2013, 117, 14019-14027.	1.1	40
107	Indirect Dynamics in a Highly Exoergic Substitution Reaction. Journal of the American Chemical Society, 2013, 135, 4250-4259.	6.6	94
108	Accelerated direct semiclassical molecular dynamics using a compact finite difference Hessian scheme. Journal of Chemical Physics, 2013, 138, 054116.	1.2	50

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109	Simulation studies of the Clâ˙ + CH3I SN2 nucleophilic substitution reaction: Comparison with ion imaging experiments. Journal of Chemical Physics, 2013, 138, 114309.	1.2	55
110	OÂ+ÂC2H4 potential energy surface: lowest-lying singlet at the multireference level. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	5
111	Comparisons of classical chemical dynamics simulations of the unimolecular decomposition of classical and quantum microcanonical ensembles. Journal of Chemical Physics, 2012, 136, 184110.	1.2	13
112	Potential energy surface for dissociation including spinâ€“orbit effects. Molecular Physics, 2012, 110, 2599-2609.	0.8	6
113	Mechanism of Thiolate-Disulfide Exchange: Additionâ€“Elimination or Effectively S_N2? Effect of a Shallow Intermediate in Gas-Phase Direct Dynamics Simulations. Journal of Physical Chemistry A, 2012, 116, 11492-11499.	1.1	16
114	Reaction dynamics of temperature-variable anion water clusters studied with crossed beams and by direct dynamics. Faraday Discussions, 2012, 157, 41.	1.6	53
115	Collision induced dissociation of doubly-charged ions: Coulomb explosion vs. neutral loss in [Ca(urea)]2+ gas phase unimolecular reactivity via chemical dynamics simulations. Physical Chemistry Chemical Physics, 2012, 14, 11724.	1.3	25
116	Gas-Phase Chemical Dynamics Simulations on the Bifurcating Pathway of the Pimaradienyl Cation Rearrangement: Role of Enzymatic Steering in Abietic Acid Biosynthesis. Journal of Chemical Theory and Computation, 2012, 8, 1212-1222.	2.3	46
117	Strikingly Different Effects of Hydrogen Bonding on the Photodynamics of Individual Nucleobases in DNA: Comparison of Guanine and Cytosine. Journal of the American Chemical Society, 2012, 134, 13662-13669.	6.6	31
118	Scattering of High-Incident-Energy Kr and Xe from Ice: Evidence that a Major Channel Involves Penetration into the Bulk. Journal of Physical Chemistry C, 2012, 116, 14264-14273.	1.5	11
119	Direct dynamics simulation of dioxetane formation and decomposition via the singlet Â·Oâ€“Oâ€“CH2â€“CH2Â· biradical: Non-RRKM dynamics. Journal of Chemical Physics, 2012, 137, 044305.	1.2	22
120	Direct dynamics determination of the reaction pathways for decomposition of the cross-linked epoxy resin constituent CH3NHCHCHCH3. Computational and Theoretical Chemistry, 2012, 990, 62-66.	1.1	4
121	UV Absorption Spectrum of Alternating DNA Duplexes. Analysis of Excitonic and Charge Transfer Interactions. Journal of Physical Chemistry A, 2012, 116, 11151-11160.	1.1	70
122	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.	1.1	139
123	OÂ+ÂC2H4 potential energy surface: excited states and biradicals at the multireference level. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	8
124	Intermolecular potentials for simulations of collisions of SiNCS+ and (CH3)2SiNCS+ ions with fluorinated self-assembled monolayers. Chemical Physics, 2012, 399, 193-204.	0.9	8
125	Homoleptic tris(methoxydimethylsilyl)silanides of the alkaline earth metals: first zwitterionic silanides with two naked silyl anions. Chemical Communications, 2011, 47, 11089.	2.2	16
126	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.	6.6	69

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127	Algorithms for Sampling a Quantum Microcanonical Ensemble of Harmonic Oscillators at Potential Minima and Conical Intersections. Journal of Physical Chemistry A, 2011, 115, 6603-6609.	1.1	29
128	Use of Direct Dynamics Simulations to Determine Unimolecular Reaction Paths and Arrhenius Parameters for Large Molecules. Journal of Chemical Theory and Computation, 2011, 7, 3478-3483.	2.3	29
129	Effect of Carbon Chain Length on the Dynamics of Heat Transfer at a Gold/Hydrocarbon Interface: Comparison of Simulation with Experiment. Journal of Physical Chemistry C, 2011, 115, 9622-9628.	1.5	21
130	Collision induced dissociation of protonated urea with N2: Effects of rotational energy on reactivity and energy transfer via chemical dynamics simulations. International Journal of Mass Spectrometry, 2011, 308, 289-298.	0.7	26
131	A Model DMMP/TiO2 (110) Intermolecular Potential Energy Function Developed from ab Initio Calculations. Journal of Physical Chemistry C, 2011, 115, 12403-12413.	1.5	22
132	Fragmentation and reactivity in collisions of protonated diglycine with chemically modified perfluorinated alkylthiolate-self-assembled monolayer surfaces. Journal of Chemical Physics, 2011, 134, 094106.	1.2	37
133	Singlet and triplet potential surfaces for the O2+C2H4 reaction. Journal of Chemical Physics, 2010, 133, 184306.	1.2	17
134	Comparisons of classical and Wigner sampling of transition state energy levels for quasiclassical trajectory chemical dynamics simulations. Journal of Chemical Physics, 2010, 133, 044313.	1.2	49
135	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.	1.1	55
136	Tribute to the Research and Professional Career of Reinhard Schinke. Journal of Physical Chemistry A, 2010, 114, 9589-9590.	1.1	0
137	Chemical Dynamics Simulations of CO₂in the Ground and First Excited Bend States Colliding with a Perfluorinated Self-Assembled Monolayer. Journal of Physical Chemistry C, 2010, 114, 18455-18464.	1.5	12
138	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.	2.1	103
139	Higher-accuracy schemes for approximating the Hessian from electronic structure calculations in chemical dynamics simulations. Journal of Chemical Physics, 2010, 133, 074101.	1.2	35
140	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.	1.3	18
141	Importance of shattering fragmentation in the surface-induced dissociation of protonated octaglycine. Journal of the American Society for Mass Spectrometry, 2009, 20, 939-948.	1.2	44
142	Bent out of shape. Nature Chemistry, 2009, 1, 103-104.	6.6	17
143	Theoretical and Computational Studies of Non-RRKM Unimolecular Dynamics. Journal of Physical Chemistry A, 2009, 113, 2236-2253.	1.1	146
144	NH₄⁺ + CH₄ Gas Phase Collisions as a Possible Analogue to Protonated Peptide/Surface Induced Dissociation. Journal of Physical Chemistry A, 2009, 113, 7543-7547.	1.1	6

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145	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.	6.6	49
146	Protonated Urea Collision-Induced Dissociation. Comparison of Experiments and Chemical Dynamics Simulations. Journal of Physical Chemistry A, 2009, 113, 13853-13862.	1.1	60
147	O(³P) + C₂H₄ Potential Energy Surface: Study at the Multireference Level. Journal of Physical Chemistry A, 2009, 113, 12663-12674.	1.1	21
148	Quantum Chemical Calculations of the Cl^{â˜'} + CH₃I â†' CH₃Cl + I^{â˜'} Potential Energy Surface. Journal of Physical Chemistry A, 2009, 113, 1976-1984.	1.1	29
149	Solvation of Dimethyl Succinate in a Sodium Hydroxide Aqueous Solution. A Computational Study. Journal of Physical Chemistry B, 2009, 113, 6473-6477.	1.2	8
150	Theoretical Investigation of Mechanisms for the Gas-Phase Unimolecular Decomposition of DMMP. Journal of Physical Chemistry A, 2009, 113, 13762-13771.	1.1	33
151	Cyclohexane Isomerization. Unimolecular Dynamics of the Twist-Boat Intermediate. Journal of Physical Chemistry A, 2009, 113, 4570-4580.	1.1	35
152	Dynamics of CO₂ Scattering off a Perfluorinated Self-Assembled Monolayer. Influence of the Incident Collision Energy, Mass Effects, and Use of Different Surface Models. Journal of Physical Chemistry A, 2009, 113, 3850-3865.	1.1	45
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