William Hase

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/2662968/publications.pdf

Version: 2024-02-01

400	18,756	12328	27402
papers	citations	69 h-index	106 g-index

437	437	437	5436
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Unimolecular Reaction Dynamics. , 1996, , .		1,002
2	Current status of transition-state theory. The Journal of Physical Chemistry, 1983, 87, 2664-2682.	2.9	745
3	Vectorization of the general Monte Carlo classical trajectory program VENUS. Journal of Computational Chemistry, 1991, 12, 1014-1024.	3.3	366
4	A SN2 Reaction That Avoids Its Deep Potential Energy Minimum. Science, 2002, 296, 875-878.	12.6	357
5	On nonâ€RRKM unimolecular kinetics: Molecules in general, and CH3NC in particular. Journal of Chemical Physics, 1973, 59, 4621-4632.	3.0	315
6	Imaging Nucleophilic Substitution Dynamics. Science, 2008, 319, 183-186.	12.6	307
7	Simulations of Gas-Phase Chemical Reactions: Applications to SN2 Nucleophilic Substitution. Science, 1994, 266, 998-1002.	12.6	284
8	Ab initio classical trajectories on the Bornâ€“Oppenheimer surface: Hessian-based integrators using fifth-order polynomial and rational function fits. Journal of Chemical Physics, 1999, 111, 3800-3805.	3.0	276
9	Ab initio classical trajectory study of H2COâ†'H2+CO dissociation. Chemical Physics Letters, 1994, 228, 436-442.	2.6	198
10	Variational unimolecular rate theory. Accounts of Chemical Research, 1983, 16, 258-264.	15.6	180
11	A simple model for correcting the zero point energy problem in classical trajectory simulations of polyatomic molecules. Journal of Chemical Physics, 1989, 91, 2863-2868.	3.0	176
12	Monte Carlo Sampling for Classical Trajectory Simulations. Advances in Chemical Physics, 2007, , 171-201.	0.3	158
13	Classical trajectory simulations of post-transition state dynamics. International Reviews in Physical Chemistry, 2008, 27, 361-403.	2.3	147
14	Theoretical and Computational Studies of Non-RRKM Unimolecular Dynamics. Journal of Physical Chemistry A, 2009, 113, 2236-2253.	2.5	146
15	Rethinking the S _N 2 reaction. Science, 2016, 352, 32-33.	12.6	146
16	DIRECT DYNAMICS SIMULATIONS OF REACTIVE SYSTEMS. , 1998, , 143-189.		143
17	Trajectory studies of SN2 nucleophilic substitution. I. Dynamics of Clâ^'+CH3Cl reactive collisions. Journal of Chemical Physics, 1990, 93, 7962-7980.	3.0	140
18	Trajectory studies ofSN2 nucleophilic substitution. II. Nonstatistical central barrier recrossing in the Clâ^'+CH3Cl system. Journal of Chemical Physics, 1992, 96, 8275-8287.	3.0	139

#	Article	IF	Citations
19	Ab Initio Study of the Interaction of Water with Cluster Models of the Aluminum Terminated (0001) Î±-Aluminum Oxide Surface. Journal of Physical Chemistry B, 1998, 102, 6539-6548.	2.6	139
20	A Direct Dynamics Trajectory Study of F⁻+ CH₃OOH Reactive Collisions Reveals a Major Non-IRC Reaction Path. Journal of the American Chemical Society, 2007, 129, 9976-9985.	13.7	139
21	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
22	On the dynamics of state selected unimolecular reactions: Chloroacetylene dissociation and predissociation. Journal of Chemical Physics, 1977, 66, 1523-1533.	3.0	128
23	Direct Chemical Dynamics Simulations. Journal of the American Chemical Society, 2017, 139, 3570-3590.	13.7	128
24	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
25	Monte carlo sampling of a microcanonical ensemble of classical harmonic oscillators. Chemical Physics Letters, 1980, 74, 284-287.	2.6	120
26	Thermal rate constant for hydrogen atom + methyl radical .fwdarw. methane recombination. 3. Comparison of experiment and canonical variational transition state theory. Journal of the American Chemical Society, 1987, 109, 2916-2922.	13.7	119
27	Classical mechanics of intramolecular vibrational energy flow in benzene. IV. Models with reduced dimensionality. Journal of Chemical Physics, 1988, 89, 6723-6735.	3.0	118
28	Some Recent Advances and Remaining Questions Regarding Unimolecular Rate Theory. Accounts of Chemical Research, 1998, 31, 659-665.	15.6	118
29	Direct Dynamics Simulations of Collision- and Surface-Induced Dissociation of N-Protonated Glycine. Shattering Fragmentationâ€. Journal of Physical Chemistry A, 2002, 106, 9983-9992.	2.5	115
30	Born-Oppenheimer Direct Dynamics Classical Trajectory Simulations. Reviews in Computational Chemistry, 2003, , 79-146.	1.5	108
31	Complete multidimensional analytic potential energy surface for chloride + chloroform SN2 nucleophilic substitution. The Journal of Physical Chemistry, 1990, 94, 2778-2788.	2.9	107
32	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
33	Direct Dynamics Study of the Stereomutation of Cyclopropane. Journal of the American Chemical Society, 1997, 119, 5251-5252.	13.7	101
34	A direct mechanism for SN2 nucleophilic substitution enhanced by mode-selective vibrational excitation. Journal of the American Chemical Society, 1989, 111, 2349-2351.	13.7	99
35	Direct Dynamics Simulation of the Lifetime of Trimethylene. Journal of the American Chemical Society, 1996, 118, 9922-9931.	13.7	98
36	The criterion of minimum state density in unimolecular rate theory. An application to ethane dissociation. Journal of Chemical Physics, 1976, 64, 2442.	3.0	97

#	Article	IF	Citations
37	Dynamics of ethyl radical decomposition. II. Applicability of classical mechanics to large-molecule unimolecular reaction dynamics. Journal of Computational Chemistry, 1982, 3, 335-343.	3.3	97
38	Trajectory Studies of SN2 Nucleophilic Substitution. 8. Central Barrier Dynamics for Gas Phase Cl-+ CH3Cl. Journal of the American Chemical Society, 2001, 123, 5753-5756.	13.7	97
39	Analytic function for the atomic hydrogen + methyl .dblarw. methane (H + CH3 .dblarw. CH4) potential energy surface. The Journal of Physical Chemistry, 1984, 88, 1339-1347.	2.9	94
40	Comparison of models for calculating the RRKM unimolecular rate constant k(E, J). Chemical Physics Letters, 1990, 175, 117-124.	2.6	94
41	Trajectory Studies of SN2 Nucleophilic Substitution. 4. Intramolecular and Unimolecular Dynamics of the Cl----CH3Br and ClCH3---Br- Complexes. Journal of the American Chemical Society, 1994, 116, 9644-9651.	13.7	94
42	Indirect Dynamics in a Highly Exoergic Substitution Reaction. Journal of the American Chemical Society, 2013, 135, 4250-4259.	13.7	94
43	Direct chemical dynamics simulations: coupling of classical and quasiclassical trajectories with electronic structure theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 296-316.	14.6	93
44	The VENUS/NWChem software package. Tight coupling between chemical dynamics simulations and electronic structure theory. Computer Physics Communications, 2014, 185, 1074-1080.	7.5	93
45	Reaction Products with Internal Energy beyond the Kinematic Limit Result from Trajectories Far from the Minimum Energy Path:Â An Example from H + HBr â†' H2+ Br. Journal of the American Chemical Society, 2005, 127, 16368-16369.	13.7	90
46	Energy transfer in rare gas collisions with self-assembled monolayers. Journal of Chemical Physics, 1997, 107, 9677-9686.	3.0	88
47	Unimolecular dynamics of Clâ^'...CH3Cl intermolecular complexes formed by Clâ^'+CH3Cl association. Journal of Chemical Physics, 1995, 102, 5626-5635.	3.0	86
48	Dynamics of Energy Transfer in Peptideâ^'Surface Collisions. Journal of the American Chemical Society, 2002, 124, 1524-1531.	13.7	84
49	Ab Initio Direct Dynamics Study of Cyclopropyl Radical Ring-Opening. Journal of the American Chemical Society, 2002, 124, 3208-3209.	13.7	83
50	Non-RRKM kinetics in gas-phase SN2 nucleophilic substitution. The Journal of Physical Chemistry, 1990, 94, 6148-6150.	2.9	82
51	Direct Dynamics Quasiclassical Trajectory Study of the Thermal Stereomutations of Cyclopropane. Journal of Physical Chemistry A, 1998, 102, 3648-3658.	2.5	82
52	Ab Initio Direct Dynamics Trajectory Study of the Cl-+ CH3Cl SN2 Reaction at High Reagent Translational Energy. Journal of the American Chemical Society, 1999, 121, 7124-7129.	13.7	81
53	Origin of the Boltzmann translational energy distribution in the scattering of hyperthermal Ne atoms off a self-assembled monolayer. Physical Chemistry Chemical Physics, 2000, 2, 901-910.	2.8	81
54	Trajectory Studies of SN2 Nucleophilic Substitution. 6. Translational Activation of the Cl-+ CH3Cl Reaction. Journal of Physical Chemistry A, 1998, 102, 6208-6214.	2.5	79

#	Article	IF	Citations
55	Trajectory studies of SN2 nucleophilic substitution. III. Dynamical stereochemistry and energy transfer pathways for the Clâ˙+CH3Cl association and direct substitution reactions. Journal of Chemical Physics, 1993, 98, 8626-8639.	3.0	78
56	Collisional Activation of Small Peptides. Journal of Physical Chemistry A, 1999, 103, 3981-3990.	2.5	78
57	Temperature Dependence of the Rate Constants and Branching Ratios for the Reactions of Cl-(D2O)1-3 with CH3Br and Thermal Dissociation Rates for Cl-(CH3Br). Journal of the American Chemical Society, 1997, 119, 577-584.	13.7	76
58	Dynamics of ethyl radical decomposition. 3. Effect of chemical activation vs. microcanonical sampling. The Journal of Physical Chemistry, 1983, 87, 2754-2763.	2.9	75
59	Modification of the Duchovicâ€“Haseâ€“Schlegel potential energy function for H+CH3â†”CH4. Comparison of canonical variational transition state theory, trajectory, and experimental association rate constants. Journal of Chemical Physics, 1991, 95, 8073-8082.	3.0	75
60	Semiempirical MNDO, AM1, and PM3 direct dynamics trajectory studies of formaldehyde unimolecular dissociation. Journal of Chemical Physics, 1996, 104, 7882-7894.	3.0	74
61	Classical dynamics simulations of SiMe3+ ionâ€“surface scattering. Journal of Chemical Physics, 1997, 106, 10337-10348.	3.0	74
62	Kinetics of F-+ CH3Cl SN2 Nucleophilic Substitution. Journal of the American Chemical Society, 1997, 119, 3093-3102.	13.7	74
63	Statistical Rate Theory Calculations of the Cl- + CH3Br .fwdarw. ClCH3 + Br- Rate Constant Versus Temperature, Translational Energy, and H(D) Isotopic Substitution. Journal of the American Chemical Society, 1995, 117, 9347-9356.	13.7	73
64	Statistical anharmonic unimolecular rate constants for the dissociation of fluxional molecules: Application to aluminum clusters. Journal of Chemical Physics, 1996, 105, 7432-7447.	3.0	73
65	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.	2.5	73
66	Theoretical Critical Configuration for Ethane Decomposition and Methyl Radical Recombination. Journal of Chemical Physics, 1972, 57, 730-733.	3.0	72
67	Quasiperiodic trajectories for a multidimensional anharmonic classical Hamiltonian excited above the unimolecular threshold. Journal of Chemical Physics, 1980, 73, 3779-3790.	3.0	72
68	Unimolecular and intramolecular dynamics. Relationship to potential energy surface properties. The Journal of Physical Chemistry, 1986, 90, 365-374.	2.9	71
69	Role of Surface Intramolecular Dynamics in the Efficiency of Energy Transfer in Ne Atom Collisions with an-Hexylthiolate Self-Assembled Monolayerâ€. Journal of Physical Chemistry A, 2003, 107, 10600-10607.	2.5	71
70	Chemical Dynamics Simulations of CO2Scattering off a Fluorinated Self-Assembled Monolayer Surface. Journal of Physical Chemistry C, 2007, 111, 354-364.	3.1	71
71	Thermal rate constant for H+CH3â€‰â†’â€‰CH4 recombination. Comparison of quasiclassical trajectory and variational transition state theory. Journal of Chemical Physics, 1985, 83, 3448-3453.	3.0	70
72	UV Absorption Spectrum of Alternating DNA Duplexes. Analysis of Excitonic and Charge Transfer Interactions. Journal of Physical Chemistry A, 2012, 116, 11151-11160.	2.5	70

#	Article	IF	Citations
73	Comparisons of Models for Simulating Energy Transfer in Ne-Atom Collisions with an Alkyl Thiolate Self-Assembled Monolayerâ€. Journal of Physical Chemistry B, 2002, 106, 8029-8037.	2.6	69
74	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
75	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.	13.7	69
76	Translational and vibrational energy dependence of the cross section for H + C2H4 .fwdarw. C2H5*. The Journal of Physical Chemistry, 1981, 85, 958-968.	2.9	68
77	Ab initio potential energy curve for CH bond dissociation in methane. Chemical Physics Letters, 1982, 89, 120-125.	2.6	68
78	Comparison of models for treating angular momentum in RRKM calculations with vibrator transition states: pressure and temperature dependence of chlorine atom + acetylene association. The Journal of Physical Chemistry, 1993, 97, 311-322.	2.9	68
79	Classical trajectory calculation of the benzene overtone spectra. The Journal of Physical Chemistry, 1988, 92, 3217-3225.	2.9	67
80	Classical mechanics of intramolecular vibrational energy flow in benzene. V. Effect of zeroâ€point energy motion. Journal of Chemical Physics, 1989, 91, 7490-7497.	3.0	67
81	The role of state specificity in unimolecular rate theory. Chemical Physics, 1989, 139, 1-13.	1.9	67
82	A Model Multidimensional Analytic Potential Energy Function for the Cl- + CH3Br .fwdarw. ClCH3 + Br- Reaction. The Journal of Physical Chemistry, 1994, 98, 1608-1619.	2.9	66
83	An ab Initio Study of the Transition State and Forward and Reverse Rate Constants for C2H5â‡Œ H + C2H4. The Journal of Physical Chemistry, 1996, 100, 5354-5361.	2.9	66
84	Trajectory Studies of SN2 Nucleophilic Substitution. 5. Semiempirical Direct Dynamics of Cl−Â·Â·CH3Br Unimolecular Decomposition. Journal of the American Chemical Society, 1996, 118, 2257-2266.	13.7	65
85	RRKM and non-RRKM behavior in chemical activation and related studies. The Journal of Physical Chemistry, 1984, 88, 6717-6720.	2.9	64
86	Trajectory studies of model Hâ€“Câ€“Câ†'H+C=C dissociation. I. Random vibrational excitation. Journal of Chemical Physics, 1980, 72, 316-331.	3.0	63
87	Perspective: chemical dynamics simulations of non-statistical reaction dynamics. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2017, 375, 20160204.	3.4	63
88	An analytic function describing the H+C2H4?C2H5 potential energy surface. Journal of Chemical Physics, 1978, 69, 3548-3562.	3.0	62
89	Trajectory studies of the molecular dynamics of ethyl radical decomposition. Journal of Chemical Physics, 1979, 71, 2911.	3.0	61
90	Analysis and extension of a model for constraining zeroâ€point energy flow in classical trajectory simulations. Journal of Chemical Physics, 1994, 100, 1179-1189.	3.0	61

#	Article	IF	Citations
91	Trajectory Studies of SN2 Nucleophilic Substitution. 7. F- + CH3Cl â†' FCH3 + Cl-. Journal of Physical Chemistry A, 1998, 102, 9819-9828.	2.5	61
92	Identifying trapping desorption in gasâ€"surface scattering. Chemical Physics Letters, 2000, 329, 84-91.	2.6	61
93	Effect of surface stiffness on the efficiency of surface-induced dissociation. Physical Chemistry Chemical Physics, 2001, 3, 2306-2314.	2.8	60
94	Molecular Dynamics Simulation of Nanoparticle Self-Assembly at a Liquidâ^'Liquid Interface. Langmuir, 2006, 22, 6385-6390.	3.5	60
95	Protonated Urea Collision-Induced Dissociation. Comparison of Experiments and Chemical Dynamics Simulations. Journal of Physical Chemistry A, 2009, 113, 13853-13862.	2.5	60
96	Role of angular momentum in statistical unimolecular rate theory. International Reviews in Physical Chemistry, 1991, 10, 249-286.	2.3	59
97	Post-transition state dynamics for propene ozonolysis: Intramolecular and unimolecular dynamics of molozonide. Journal of Chemical Physics, 2006, 125, 014317.	3.0	59
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.	13.7	59
99	Imaging dynamic fingerprints of competing E2 and SN2 reactions. Nature Communications, 2017, 8, 25.	12.8	59
100	Properties of canonical variational transition state theory for association reactions without potential energy barriers. The Journal of Physical Chemistry, 1989, 93, 6029-6038.	2.9	57
101	Product Energy and Angular Momentum Partitioning in the Unimolecular Dissociation Of Aluminum Clustersâ€. Journal of Physical Chemistry A, 2000, 104, 10556-10564.	2.5	57
102	1985, 82, 123-133.	3.0	56
103	Direct dynamics study of energy transfer and collision-induced dissociation: Effects of impact energy, geometry, and reactant vibrational mode in H2CO+â€"Ne collisions. Journal of Chemical Physics, 2003, 119, 3040-3050.	3.0	55
104	A washboard with moment of inertia model of gas-surface scattering. Journal of Chemical Physics, 2004, 120, 1031-1043.	3.0	55
105	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
106	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
107	The sensitivity of IVR in benzene to bendâ€"stretch potential energy coupling. Journal of Chemical Physics, 1986, 85, 4422-4426.	3.0	54
108	Fitting classical microcanonical unimolecular rate constants to a modified RRK expression: Anharmonic and variational effects. Journal of Chemical Physics, 1999, 110, 6198-6207.	3.0	53

#	Article	IF	Citations
109	Reaction dynamics of temperature-variable anion water clusters studied with crossed beams and by direct dynamics. Faraday Discussions, 2012, 157, 41.	3.2	53
110	Chemical dynamics simulations of the monohydrated OHâˆ™(H2O) + CH3I reaction. Atomic-level mechanisms and comparison with experiment. Journal of Chemical Physics, 2015, 142, 244308.	3.0	53
111	Intramolecular vibrational energy relaxation in benzene. Chemical Physics Letters, 1978, 54, 73-76.	2.6	52
112	A dynamical study of the H+CH3â†'CH4 recombination reaction. Journal of Chemical Physics, 1985, 82, 3599-3606.	3.0	52
113	Energy Transfer Dynamics in the Collision-Induced Dissociation of Al6 and Al13 Clusters. The Journal of Physical Chemistry, 1995, 99, 8147-8161.	2.9	52
114	Thresholds for the Collision-Induced Dissociation of Clusters by Rare Gas Impact. The Journal of Physical Chemistry, 1996, 100, 8190-8196.	2.9	52
115	Trajectory studies of model Hâ€“Câ€“Câ€‰â†'â€‰H+C=C dissociation. III. Details of the lifetime distribution following chemical activation. Journal of Chemical Physics, 1984, 80, 714-719.	3.0	51
116	Comparison of Explicit and United Atom Models for Alkane Chains Physisorbed on Î±-Al2O3 (0001). Journal of Physical Chemistry B, 1999, 103, 3885-3895.	2.6	51
117	Energy transfer pathways in the collisional activation of peptides. International Journal of Mass Spectrometry, 2000, 201, 233-244.	1.5	51
118	Dynamics of the biradical mediating vinylcyclopropaneâ€“cyclopentene rearrangement. Physical Chemistry Chemical Physics, 2002, 4, 304-312.	2.8	51
119	Direct dynamics study of N-protonated diglycine surface-induced dissociation. Influence of collision energy. Journal of the American Society for Mass Spectrometry, 2003, 14, 1402-1412.	2.8	51
120	Accelerated direct semiclassical molecular dynamics using a compact finite difference Hessian scheme. Journal of Chemical Physics, 2013, 138, 054116.	3.0	50
121	A comparison of classical trajectory and statistical unimolecular rate theory calculations of Al3decomposition. Journal of Chemical Physics, 1994, 101, 8535-8553.	3.0	49
122	Quantum mechanical study of the unimolecular dissociation of HO2: A rigorous test of RRKM theory. Journal of Chemical Physics, 1995, 102, 5867-5870.	3.0	49
123	Quasiclassical trajectory calculations for the OH(Xâ€‰2Î) and OD(Xâ€‰2Î)+HBr reactions: Energy partitioning and rate constants. Journal of Chemical Physics, 1996, 105, 9897-9911.	3.0	49
124	Dynamics of Energy Transfer in Collisions of O(3P) Atoms with a 1-Decanethiol Self-Assembled Monolayer Surface. Journal of Physical Chemistry B, 2006, 110, 11863-11877.	2.6	49
125	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.	13.7	49
126	Comparisons of classical and Wigner sampling of transition state energy levels for quasiclassical trajectory chemical dynamics simulations. Journal of Chemical Physics, 2010, 133, 044313.	3.0	49

#	Article	IF	Citations
127	Sum and density of states for anharmonic polyatomic molecules. Effect of bendâ€“stretch coupling. Journal of Chemical Physics, 1983, 78, 5052-5058.	3.0	48
128	Efficiency of energy transfer in protonated diglycine and dialanine SID. International Journal of Mass Spectrometry, 2003, 230, 57-63.	1.5	48
129	Quasiclassical dynamics simulation of the collision-induced dissociation of Cr(CO)6+ with Xe. Journal of Chemical Physics, 2005, 123, 154311.	3.0	48
130	Properties of Complexes Formed by Na⁺, Mg²⁺, and Fe²⁺ Binding with Benzene Molecules. Journal of Physical Chemistry A, 2014, 118, 9500-9511.	2.5	48
131	Reaction path Hamiltonian analysis of the dynamics for Clâ¯ + CH3Br â† ClCH3 + Brâ¯ SN2 nucleophilic substitution. Chemical Physics, 1996, 212, 247-258.	1.9	47
132	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
133	Trajectory studies of model Hâ€“Câ€“Câ†'H+C = C dissociation. II. Angular momenta and energy partitioning and their relation to nonâ€RRKM dynamics. Journal of Chemical Physics, 1981, 75, 3809-3820.	3.0	46
134	Resolution of a paradox concerning the forward and reverse rate constants for ethyl .dblarw. atomic hydrogen + ethylene. The Journal of Physical Chemistry, 1982, 86, 3901-3904.	2.9	46
135	Trajectory studies of S[sub N]2 nucleophilic substitution. IX. Microscopic reaction pathways and kinetics for Cl[sup â¯]+CH[sub 3]Br. Journal of Chemical Physics, 2003, 118, 2688.	3.0	46
136	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.	5.3	46
137	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
138	Dynamics of Unimolecular Reactions. , 1976, , 121-169.		45
139	Direct dynamics simulations using Hessian-based predictor-corrector integration algorithms. Journal of Chemical Physics, 2007, 126, 044105.	3.0	45
140	Chemical Dynamics Study of Intrasurface Hydrogen-Bonding Effects in Gasâ¯Surface Energy Exchange and Accommodation. Journal of Physical Chemistry C, 2008, 112, 476-490.	3.1	45
141	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.	2.5	45
142	Use of a single trajectory to study product energy partitioning in unimolecular dissociation: Mass effects for halogenated alkanes. Journal of Chemical Physics, 2006, 124, 064313.	3.0	44
143	Importance of shattering fragmentation in the surface-induced dissociation of protonated octaglycine. Journal of the American Society for Mass Spectrometry, 2009, 20, 939-948.	2.8	44
144	Evaluating the Accuracy of Hessian Approximations for Direct Dynamics Simulations. Journal of Chemical Theory and Computation, 2013, 9, 54-64.	5.3	44

#	Article	IF	Citations
145	Effect of anharmonicity on intermolecular energy transfer from highly vibrationally excited molecules. The Journal of Physical Chemistry, 1988, 92, 4040-4046.	2.9	43
146	Ab initiodirect dynamics trajectory simulation of C2H5Fâ†'C2H4+HF product energy partitioning. Journal of Chemical Physics, 2004, 121, 8831-8845.	3.0	43
147	Classical trajectory study of the unimolecular decomposition of Hâ€“Câ‰¡Câ€“Cl, Hâ€“Câ‰¡Câ€“H, and Clâ€“Câ‰¡Câ€“Cl. Journal of Chemical Physics, 1974, 61, 4690-4699.	3.0	42
148	A PM3-SRP + Analytic Function Potential Energy Surface Model for O(3P) Reactions with Alkanes. Application to O(3P) + Ethaneâ€. Journal of Physical Chemistry A, 2004, 108, 9863-9875.	2.5	42
149	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	3.0	42
150	A classical trajectory study of the F+C2H4â†'C2H4Fâ†'H+C2H3F reaction dynamics. Journal of Chemical Physics, 1981, 75, 2807-2819.	3.0	41
151	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.	2.5	40
152	A quasiclassical trajectory calculation of the atomic hydrogen + ethylene .fwdarw. ethyl bimolecular rate constant. The Journal of Physical Chemistry, 1983, 87, 4715-4720.	2.9	39
153	Effect of bond stretch excitation on the attenuation of bending forces. Chemical Physics Letters, 1986, 132, 493-497.	2.6	39
154	Kinetics of the reaction between hydroxyl and hydroperoxyl on the singlet potential energy surface. The Journal of Physical Chemistry, 1991, 95, 6784-6792.	2.9	39
155	Simulations of hydrocarbon adsorption and subsequent water penetration on an aluminum oxide surface. Journal of Chemical Physics, 1997, 106, 7331-7342.	3.0	39
156	A Hamiltonian with a Subset of Normal Modes for Studying Mode-Specific Energy Transfer in Intermolecular Collisionsâ€. Journal of Physical Chemistry A, 2001, 105, 2617-2625.	2.5	39
157	Quantum dynamical study of the Cl-+CH3Br SN2 reaction. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 737-746.	1.7	38
158	Direct Dynamics Trajectory Study of Vibrational Effects:Â Can Polanyi Rules Be Generalized to a Polyatomic System?. Journal of the American Chemical Society, 2004, 126, 8602-8603.	13.7	38
159	An ab initio direct dynamics simulation of protonated glycine surface-induced dissociation. International Journal of Mass Spectrometry, 2007, 265, 326-336.	1.5	38
160	Simulations of energy transfer in Cr(CO)6+ surface-induced dissociation. International Journal of Mass Spectrometry and Ion Processes, 1998, 174, 1-9.	1.8	37
161	Fragmentation and reactivity in collisions of protonated diglycine with chemically modified perfluorinated alkylthiolate-self-assembled monolayer surfaces. Journal of Chemical Physics, 2011, 134, 094106.	3.0	37
162	Ab initio molecular orbital studies of atomic hydrogen + ethylene and atomic fluorine + ethylene. 2. Comparison of the energetics. The Journal of Physical Chemistry, 1982, 86, 4883-4888.	2.9	36

#	Article	IF	Citations
163	Transition states and rate constants for ionâ€“molecule association. II. Li++(CH3)2Oâ†'Li+[(CH3)2O]. Journal of Chemical Physics, 1987, 86, 1348-1355.	3.0	36
164	Nascent energy distribution of the Criegee intermediate CH2OO from direct dynamics calculations of primary ozonide dissociation. Journal of Chemical Physics, 2018, 148, 174306.	3.0	36
165	Dynamics of Cr(CO)[sub 6][sup +] collisions with hydrogenated surfaces. Journal of Chemical Physics, 2003, 118, 2893.	3.0	35
166	Chemical Dynamics Simulations of Energy Transfer in Collisions of Protonated Peptideâˆ'Ions with a Perfluorinated Alkylthiol Self-Assembled Monolayer Surface. Journal of Physical Chemistry C, 2008, 112, 9377-9386.	3.1	35
167	Cyclohexane Isomerization. Unimolecular Dynamics of the Twist-Boat Intermediate. Journal of Physical Chemistry A, 2009, 113, 4570-4580.	2.5	35
168	Higher-accuracy schemes for approximating the Hessian from electronic structure calculations in chemical dynamics simulations. Journal of Chemical Physics, 2010, 133, 074101.	3.0	35
169	Potential energy surface and unimolecular dynamics of stretched n-butane. Journal of Chemical Physics, 2008, 129, 094701.	3.0	34
170	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
171	Is there hydrogen bonding for gas phase SN2 pre-reaction complexes?. International Journal of Mass Spectrometry, 2015, 378, 14-19.	1.5	34
172	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.	2.5	34
173	Dynamics of ionâ€“molecule recombination. II. An alkali ion and a water molecule. Journal of Chemical Physics, 1982, 77, 3011-3021.	3.0	33
174	Sensitivity of the H + CH3 â†' CH4 recombination rate constant to the shape of the Cî—¸H stretching potential. Chemical Physics Letters, 1984, 110, 474-477.	2.6	33
175	A potential energy function for the hydroperoxyl radical. The Journal of Physical Chemistry, 1987, 91, 1596-1602.	2.9	33
176	Direct dynamics simulations of the oxidation of a single wall carbon nanotube. Physical Chemistry Chemical Physics, 2001, 3, 4376-4383.	2.8	33
177	Stationary points for the OHâˆ' + CH3F â†' CH3OH + Fâˆ' potential energy surface. International Journal of Mass Spectrometry, 2003, 227, 315-325.	1.5	33
178	Comparison of Levels of Electronic Structure Theory in Direct Dynamics Simulations of C2H5F â†' HF + C2H4Product Energy Partitioningâ€. Journal of Physical Chemistry A, 2006, 110, 1484-1490.	2.5	33
179	Theoretical Investigation of Mechanisms for the Gas-Phase Unimolecular Decomposition of DMMP. Journal of Physical Chemistry A, 2009, 113, 13762-13771.	2.5	33
180	Ab initio potential and variational transition state theory rate constant for Hâ€atom association with the diamond (111) surface. Journal of Chemical Physics, 1994, 101, 2476-2488.	3.0	32

#	Article	IF	Citations
181	An ab initio quasi-classical direct dynamics investigation of the F+C2H4â†'C2H3F+H product energy distributions. Physical Chemistry Chemical Physics, 1999, 1, 999-1011.	2.8	32
182	Inelastic Scattering Dynamics of Ar from a Perfluorinated Self-Assembled Monolayer Surface. Journal of Physical Chemistry A, 2007, 111, 12785-12794.	2.5	32
183	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.	13.7	31
184	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
185	Steric Effects of Solvent Molecules on S_N2 Substitution Dynamics. Journal of Physical Chemistry Letters, 2017, 8, 1885-1892.	4.6	31
186	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
187	Dynamics of ion-molecule recombination. III. Trends in the recombination efficiency. Journal of the American Chemical Society, 1984, 106, 4071-4077.	13.7	30
188	A unified model for simulating liquid and gas phase, intermolecular energy transfer: N2 + C6F6 collisions. Journal of Chemical Physics, 2014, 140, 194103.	3.0	30
189	Dynamics of Protonated Peptide Ion Collisions with Organic Surfaces: Consonance of Simulation and Experiment. Journal of Physical Chemistry Letters, 2016, 7, 3142-3150.	4.6	30
190	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.	2.8	30
191	Trajectory studies of unimolecular processes. II. Dynamics of chloroacetylene dissociation. Journal of Chemical Physics, 1976, 64, 651-655.	3.0	29
192	Comparison of molecular dynamics and variational transition-state-theory calculations of the rate constant for H-atom association with the diamond {111} surface. Physical Review B, 1995, 52, 2949-2958.	3.2	29
193	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
194	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.	2.5	29
195	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.	5.3	29
196	Zero-Point Energy Constraint for Unimolecular Dissociation Reactions. Giving Trajectories Multiple Chances To Dissociate Correctly. Journal of Physical Chemistry A, 2016, 120, 372-378.	2.5	29
197	Excitation Energies of Chemically Activated Isobutane and Neopentane and the Correlation of Their Decomposition Rates with Radical Recombination Rates. Journal of Chemical Physics, 1971, 54, 1277-1283.	3.0	28
198	The decomposition of chemically activatedn-butane, isopentane, neohexane, andn-pentane and the correlation of their decomposition rates with radical recombination rates.. International Journal of Chemical Kinetics, 1972, 4, 1-35.	1.6	28

#	Article	IF	Citations
199	Ketene photochemistry. Relative CH2(1A1) quantum yields at 3130, 3340 and 3660 Ã.... Chemical Physics Letters, 1975, 35, 57-62.	2.6	28
200	Dynamics of ion solvation. Li++H2Oâ†'Li+(H2O)*. Journal of Chemical Physics, 1981, 75, 738-744.	3.0	28
201	Reaction path and variational transition state theory rate constant for Li++H2Oâ†'Li+(H2O) association. Journal of Chemical Physics, 1986, 84, 3783-3787.	3.0	28
202	Mode specificity in the model unimolecular reaction H-C-C .fwdarw. H + C:C. The Journal of Physical Chemistry, 1986, 90, 3517-3524.	2.9	28
203	Quantum and semiclassical vibrational transition frequencies for a Hamiltonian with stretchâ€"bend potential energy coupling. Journal of Chemical Physics, 1986, 84, 361-368.	3.0	28
204	A QM/MM Direct Dynamics Trajectory Investigation of Trimethylene Decomposition in an Argon Bath. Journal of Physical Chemistry B, 1999, 103, 3691-3698.	2.6	28
205	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.	38.1	28
206	Properties of variational transition states for association reactions. Chemical Physics Letters, 1987, 139, 389-394.	2.6	27
207	A direct dynamics study of the F + C2H4 â†' C2H3F + H product energy distributions. Chemical Physics Letters, 1998, 288, 621-627.	2.6	27
208	Energetics, transition states, and intrinsic reaction coordinates for reactions associated with O(3P) processing of hydrocarbon materials. Journal of Chemical Physics, 2004, 120, 9253-9265.	3.0	27
209	Kinematically complete chemical reaction dynamics. Journal of Physics: Conference Series, 2009, 194, 012046.	0.4	27
210	Unimolecular dissociation of peptides: statistical vs. non-statistical fragmentation mechanisms and time scales. Faraday Discussions, 2016, 195, 599-618.	3.2	27
211	Kinetics of Chemically Activated Isobutane and Neopentane from the 4358â€•and 3660â€Ã... Photolyses of Diazomethane with Propane and Isobutane. Journal of Chemical Physics, 1970, 52, 3911-3919.	3.0	26
212	Comparison of quantum and semiclassical variational transition state models for the HO2â†'H+O2microcanonical rate constant. Journal of Chemical Physics, 1995, 103, 8891-8900.	3.0	26
213	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.	1.5	26
214	Competing E2 and S_N2 Mechanisms for the F^{â€"} + CH₃CH₂I Reaction. Journal of Physical Chemistry A, 2017, 121, 1078-1085.	2.5	26
215	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.	2.8	25
216	Chemical Dynamics Simulations of Benzene Dimer Dissociation. Journal of Physical Chemistry A, 2015, 119, 6631-6640.	2.5	25

#	Article	IF	Citations
217	On the relationship between unimolecular lifetime and relative translational energy distributions. Chemical Physics Letters, 1979, 67, 263-266.	2.6	24
218	Dynamics of ionâ€“molecule recombination. V. A study of energy transfer pathways. Journal of Chemical Physics, 1992, 96, 8295-8306.	3.0	24
219	Surface energy transfer by low energy polyatomic ion collisions. Nuclear Instruments & Methods in Physics Research B, 1997, 125, 218-222.	1.4	24
220	Energy and temperature dependent dissociation of the Na+(benzene)1,2 clusters: Importance of anharmonicity. Journal of Chemical Physics, 2015, 142, 044306.	3.0	24
221	SYNTHESIS OF FORMAMIDE AND RELATED ORGANIC SPECIES IN THE INTERSTELLAR MEDIUM VIA CHEMICAL DYNAMICS SIMULATIONS. Astrophysical Journal, 2016, 826, 107.	4.5	24
222	Collisional deactivation of highly vibrationally excited molecules. Dynamics of the collision event. The Journal of Physical Chemistry, 1984, 88, 5135-5138.	2.9	23
223	Energy transfer in collisions of argon with highly excited water and methane. The Journal of Physical Chemistry, 1985, 89, 2502-2507.	2.9	23
224	Sensitivity of unimolecular lifetime distributions and energy dependent rate constants to fluctuations in state specific rate constants. Journal of Chemical Physics, 1989, 90, 1557-1563.	3.0	23
225	Use of microclusters to simulate cage, trapping, and chaperon effects in association reactions. The Journal of Physical Chemistry, 1992, 96, 7535-7546.	2.9	23
226	Temperature gradients and frictional energy dissipation in the sliding of hydroxylated Î±-alumina surfaces. Physical Chemistry Chemical Physics, 2002, 4, 5377-5385.	2.8	23
227	Electronic nature of zwitterionic alkali metal methanides, silanides and germanides â€“ a combined experimental and computational approach. Chemical Science, 2017, 8, 1316-1328.	7.4	23
228	A theoretical study of growth mechanism of the (110) surface of diamond from acetylene and hydrogen mixtures. The Journal of Physical Chemistry, 1992, 96, 9369-9376.	2.9	22
229	Structures, Energies, and Electrostatics for Methane Complexed with Alumina Clusters. Journal of Physical Chemistry A, 2000, 104, 4920-4927.	2.5	22
230	Ab Initio and Analytic Intermolecular Potentials for Arâ‹¯CF4. Journal of Physical Chemistry A, 2006, 110, 3174-3178.	2.5	22
231	Effects of projectile orientation and surface impact site on the efficiency of projectile excitation in surface-induced dissociation. International Journal of Mass Spectrometry, 2006, 249-250, 321-329.	1.5	22
232	Chemical Dynamics Simulation of Ne Atom Scattering off a Squalane Surface. Journal of Physical Chemistry C, 2008, 112, 20340-20346.	3.1	22
233	A Model DMMP/TiO2 (110) Intermolecular Potential Energy Function Developed from ab Initio Calculations. Journal of Physical Chemistry C, 2011, 115, 12403-12413.	3.1	22
234	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.	3.0	22

#	Article	IF	Citations
235	Bath Model for N₂ + C₆F₆ Gas-Phase Collisions. Details of the Intermolecular Energy Transfer Dynamics. Journal of Physical Chemistry C, 2015, 119, 14683-14691.	3.1	22
236	Post-Transition State Dynamics in Gas Phase Reactivity: Importance of Bifurcations and Rotational Activation. Journal of Chemical Theory and Computation, 2016, 12, 974-982.	5.3	22
237	Ethyl radical potential energy surface. Faraday Discussions of the Chemical Society, 1977, 62, 210.	2.2	21
238	Search for quasiperiodic motion in vibrationally excited formaldehyde formed by S1 â†' So internal conversion. Chemical Physics Letters, 1982, 92, 371-378.	2.6	21
239	Comparison of ab Initio and Empirical Potentials for H-Atom Association with Diamond Surfaces. The Journal of Physical Chemistry, 1996, 100, 1761-1766.	2.9	21
240	O(³P) + C₂H₄ Potential Energy Surface: Study at the Multireference Level. Journal of Physical Chemistry A, 2009, 113, 12663-12674.	2.5	21
241	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.	3.1	21
242	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.	2.8	21
243	Importance of angular momentum constraints in the product energy partitioning of model Hâ€“Câ€“Câ€“â†'H+C=C dissociation. Journal of Chemical Physics, 1980, 73, 3010-3011.	3.0	20
244	Semiclassical vibrational energy levels for a model H-C-C .fwdarw. H + C=C Hamiltonian. The Journal of Physical Chemistry, 1982, 86, 2873-2879.	2.9	20
245	Quasiclassical trajectory study of the n = 3 overtone state of benzene. Chemical Physics Letters, 1987, 142, 187-190.	2.6	20
246	Monoenergetic unimolecular rate constants and their dependence on pressure and fluctuations in state-specific unimolecular rate constants. The Journal of Physical Chemistry, 1989, 93, 1681-1683.	2.9	20
247	Dynamics and Kinetics of Heat Transfer at the Interface of Model Diamond {111} Nanosurfacesâ€. Journal of Physical Chemistry A, 2006, 110, 526-536.	2.5	20
248	Chemical Dynamics Simulations of Intermolecular Energy Transfer: Azulene + N₂ Collisions. Journal of Physical Chemistry A, 2016, 120, 5187-5196.	2.5	20
249	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
250	<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.	2.5	20
251	Nonstatistical Reaction Dynamics. Annual Review of Physical Chemistry, 2020, 71, 289-313.	10.8	20
252	The calculation and interpretation of average collisional energy transfer parameters. Chemical Physics Letters, 1988, 152, 377-381.	2.6	19

#	Article	IF	Citations
253	Comparison of zeroâ€point energy constrained and quantum anharmonic Riceâ€“Ramspergerâ€“Kasselâ€“Marcus and phase space theory rate constants for Al3dissociation. Journal of Chemical Physics, 1996, 104, 9445-9460.	3.0	19
254	The Fâ¯+ CH3I â† FCH3+ Iâ¯ entrance channel potential energy surface. International Journal of Mass Spectrometry, 2015, 377, 222-227.	1.5	19
255	Gas Phase Synthesis of Protonated Glycine by Chemical Dynamics Simulations. Journal of Physical Chemistry A, 2018, 122, 869-877.	2.5	19
256	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.	3.0	19
257	Chemical Dynamics Simulations and Scattering Experiments for O₂ Collisions with Graphite. Journal of Physical Chemistry C, 2018, 122, 16048-16059.	3.1	19
258	A bimolecular mechanism for ketene photodissociation in the near ultraviolet. Journal of Chemical Physics, 1977, 66, 5093-5099.	3.0	18
259	Reaction path and kinetics for sodium(1+) complexation with 18-crown-6. The Journal of Physical Chemistry, 1989, 93, 539-545.	2.9	18
260	Transition state dynamics and a QM/MM model for the ClÂ– + C2H5Cl SN2 reaction. Canadian Journal of Chemistry, 2004, 82, 891-899.	1.1	18
261	Intermolecular Potential To Represent Collisions of Protonated Peptide Ions with Fluorinated Alkane Surfacesâ€. Journal of Physical Chemistry B, 2005, 109, 8320-8324.	2.6	18
262	Direct Dynamics Trajectory Study of the Reaction of Formaldehyde Cation with D2:Â Vibrational and Zero-Point Energy Effects on Quasiclassical Trajectoriesâ€. Journal of Physical Chemistry A, 2005, 109, 11376-11384.	2.5	18
263	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.	2.8	18
264	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.	3.1	18
265	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.	3.4	18
266	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.	2.5	18
267	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.	2.8	18
268	Kinetics of chemically activated ethane. International Journal of Chemical Kinetics, 1973, 5, 77-92.	1.6	17
269	A model analytic potential energy function for formyl radical decomposition. The Journal of Physical Chemistry, 1990, 94, 7371-7377.	2.9	17
270	Central barrier recrossing dynamics of the Clâ¯+CD3Cl SN2 reaction. Computational and Theoretical Chemistry, 2006, 771, 27-31.	1.5	17

#	Article	IF	Citations
271	Bent out of shape. Nature Chemistry, 2009, 1, 103-104.	13.6	17
272	Singlet and triplet potential surfaces for the O2+C2H4 reaction. Journal of Chemical Physics, 2010, 133, 184306.	3.0	17
273	Intermolecular Potential for Binding of Protonated Peptide Ions with Perfluorinated Hydrocarbon Surfaces. Journal of Physical Chemistry B, 2014, 118, 5577-5588.	2.6	17
274	Chemical Dynamics Simulation of Low Energy N₂ Collisions with Graphite. Journal of Physical Chemistry C, 2018, 122, 612-623.	3.1	17
275	Dynamics of Pyrene-Dimer Association and Ensuing Pyrene-Dimer Dissociation. Journal of Physical Chemistry A, 2020, 124, 8907-8917.	2.5	17
276	Unimolecular processes in weakly bound complexes: correlated product state distributions. Faraday Discussions, 1995, 102, 323.	3.2	16
277	Direct Dynamics Studies of CO-Assisted Carbon Nanotube Growth. Journal of Physical Chemistry B, 2002, 106, 12418-12425.	2.6	16
278	Homoleptic tris(methoxydimethylsilyl)silanides of the alkaline earth metals: first zwitterionic silanides with two naked silyl anions. Chemical Communications, 2011, 47, 11089.	4.1	16
279	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.	2.5	16
280	Direct Dynamics Simulation of Dissociation of the [CH₃--I--OH]^{â^'} Ionâ€“Molecule Complex. Journal of Physical Chemistry A, 2015, 119, 817-825.	2.5	16
281	Chemically activated methylcyclobutane exothermicity of singlet methylene reactions and the heat of formation of singlet methylene. International Journal of Chemical Kinetics, 1975, 7, 879-894.	1.6	15
282	Semiclassical vibrational eigenvalues of a threeâ€dimensional Hamiltonian. Journal of Chemical Physics, 1984, 80, 1462-1468.	3.0	15
283	An analytical potential energy function to model protonated peptide soft-landing experiments. The CH3NH3+/CH4 interactions. Physical Chemistry Chemical Physics, 2008, 10, 4565.	2.8	15
284	Dynamics of Na+(Benzene) + Benzene Association and Ensuing Na+(Benzene)2* Dissociation. Journal of Physical Chemistry A, 2015, 119, 7894-7904.	2.5	15
285	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.	2.5	15
286	Non-statistical intermolecular energy transfer from vibrationally excited benzene in a mixed nitrogen-benzene bath. Journal of Chemical Physics, 2018, 149, 134101.	3.0	15
287	Decomposition kinetics of chemically activated dimethylsilane and ethylsilane. Journal of the American Chemical Society, 1973, 95, 3454-3459.	13.7	14
288	Exit-channel coupling effects in the unimolecular decomposition of triatomics. The Journal of Physical Chemistry, 1979, 83, 933-936.	2.9	14

#	Article	IF	Citations
289	On non-exponential unimolecular dissociation of molecules prepared by vibrational overtone excitation. Chemical Physics Letters, 1985, 116, 312-316.	2.6	14
290	Dynamics of Ar+CH[sub 4]/Ni{111} collision-induced desorption. Journal of Chemical Physics, 2001, 114, 535.	3.0	14
291	Nonequilibrium energy dissipation at the interface of sliding model hydroxylated Î±-alumina surfaces. Journal of Chemical Physics, 2005, 122, 094713.	3.0	14
292	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.	3.0	14
293	Chemical Dynamics Simulations of Energy Transfer for Propylbenzene Cation and He Collisions. Journal of Physical Chemistry A, 2017, 121, 7494-7502.	2.5	14
294	Chemically Activated Tetramethylsilane from the Reaction of Singlet Methylene Radicals with Trimethylsilane. Journal of Chemical Physics, 1970, 52, 4004-4010.	3.0	13
295	Importance of energy transfer and lattice properties in hydrogen-atom association with the (111) surface of diamond. The Journal of Physical Chemistry, 1993, 97, 9934-9941.	2.9	13
296	An analytic hindered rotor model for calculating microcanonical variational unimolecular rate constants from reaction path properties. International Journal of Chemical Kinetics, 1994, 26, 407-419.	1.6	13
297	Effect of Surface Stiffness on the Friction of Sliding Model Hydroxylated Î±-Alumina Surfaces. Journal of Physical Chemistry B, 2001, 105, 12032-12045.	2.6	13
298	Relationship between Mode Specific and Thermal Unimolecular Rate Constants for HOCl â†' OH + Cl Dissociation. Journal of Physical Chemistry A, 2002, 106, 8339-8344.	2.5	13
299	Comparisons of classical chemical dynamics simulations of the unimolecular decomposition of classical and quantum microcanonical ensembles. Journal of Chemical Physics, 2012, 136, 184110.	3.0	13
300	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.	2.8	13
301	Exploratory Direct Dynamics Simulations of ³O₂ Reaction with Graphene at High Temperatures. Journal of Physical Chemistry C, 2018, 122, 29368-29379.	3.1	13
302	Threshold for shattering fragmentation in collision-induced dissociation of the doubly protonated tripeptide TIK(H⁺)₂. Physical Chemistry Chemical Physics, 2018, 20, 19744-19749.	2.8	13
303	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.	3.0	13
304	Comparison of canonical variational transition state theory rate constants for hydrogen atom association with alkyl radicals and with the (111) surface of diamond. The Journal of Physical Chemistry, 1993, 97, 11706-11711.	2.9	12
305	Lyapunov exponents for the intramolecular motion of the Clâ‹¯CH3Br complex. International Journal of Mass Spectrometry and Ion Processes, 1997, 167-168, 573-585.	1.8	12
306	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.	3.1	12

#	Article	IF	Citations
307	Direct Dynamics Simulation of the Activation and Dissociation of 1,5-Dinitrobiuret (HDNB). Journal of Physical Chemistry A, 2014, 118, 2228-2236.	2.5	12
308	Direct dynamics simulations of the unimolecular dissociation of dioxetane: Probing the non-RRKM dynamics. Journal of Chemical Physics, 2018, 148, 164309.	3.0	12
309	Dynamic of gas-phase SN2 nucleophilic substitution reactions. Advances in Gas Phase Ion Chemistry, 1998, , 125-156.	0.8	12
310	Linear Free Energy of Activation Relationship for Barrierless Association Reactions. Journal of the American Chemical Society, 1997, 119, 5007-5012.	13.7	11
311	Isomerisation of deuterated cyclopropanes â€" The possibility for stereochemical control. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1997, 101, 414-422.	0.9	11
312	Role of State Specificity in the Temperature- and Pressure-Dependent Unimolecular Rate Constants for HO2â† H + O2Dissociation. Journal of Physical Chemistry A, 1998, 102, 1292-1296.	2.5	11
313	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.	3.1	11
314	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.	3.1	11
315	Understanding Energy Transfer in Gasâ€"Surface Collisions from Gas-Phase Models. Journal of Physical Chemistry C, 2014, 118, 2609-2621.	3.1	11
316	Direct Dynamics Simulation of the Thermal 3CH2 + 3O2 Reaction. Rate Constant and Product Branching Ratios. Journal of Physical Chemistry A, 2018, 122, 4808-4818.	2.5	11
317	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.	1.5	11
318	Kinetics of vibrationally hot propane produced by methylene insertion into ethane. The Journal of Physical Chemistry, 1972, 76, 607-614.	2.9	10
319	Rice-Ramsperger-Kassel-Marcus Theory Applied to Decomposition of Hot Atom Substitution Products. c-C4H7T and c-C4D7T. The Journal of Physical Chemistry, 1974, 78, 2309-2315.	2.9	10
320	Classical number and density of states. Journal of Chemical Education, 1983, 60, 379.	2.3	10
321	A semi-empirical canonical variational transition state theory model for association reactions without potential energy barriers. Chemical Physics Letters, 1989, 156, 115-118.	2.6	10
322	Role of Projectile and Surface Temperatures in the Energy Transfer Dynamics of Protonated Peptide Ion Collisions with the Diamond {111} Surfaceâ€. Journal of Physical Chemistry A, 2006, 110, 8418-8422.	2.5	10
323	Theoretical Study of the Dynamics of the HBr⁺ + CO₂ â† HOCO⁺ + Br Reaction. Journal of Physical Chemistry A, 2020, 124, 9119-9127.	2.5	10
324	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.	3.1	10

#	Article	IF	Citations
325	Comparison of methylene radical insertion reactions with the Si-H bonds of methylsilane, dimethylsilane, and trimethylsilane. The Journal of Physical Chemistry, 1969, 73, 4401-4403.	2.9	9
326	Ab initio and analytic intermolecular potentials for Arâ€“CH3OH. Physical Chemistry Chemical Physics, 2006, 8, 4678-4684.	2.8	9
327	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.	2.5	9
328	Chemical Dynamics Simulation of Energy Transfer: Propylbenzene Cation and N₂ Collisions. Journal of Physical Chemistry A, 2019, 123, 2301-2309.	2.5	9
329	Trajectory study of energy partition in CF3CN â†' CF3 + CN dissociation dynamics. Chemical Physics, 1986, 110, 27-39.	1.9	8
330	Dynamics of ion-molecule recombination IV. Li+ + (CH3)2O association. Computer Physics Communications, 1988, 51, 17-34.	7.5	8
331	Computer simulation of sliding hydroxylated alumina surfaces. Tribology Letters, 1999, 7, 153-159.	2.6	8
332	Solvation of Dimethyl Succinate in a Sodium Hydroxide Aqueous Solution. A Computational Study. Journal of Physical Chemistry B, 2009, 113, 6473-6477.	2.6	8
333	OÂ+ÂC2H4 potential energy surface: excited states and biradicals at the multireference level. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	8
334	Intermolecular potentials for simulations of collisions of SiNCS+ and (CH3)2SiNCS+ ions with fluorinated self-assembled monolayers. Chemical Physics, 2012, 399, 193-204.	1.9	8
335	Models for Intrinsic Non-RRKM Dynamics. Decomposition of the SN2 Intermediate Clâ€“â€“CH3Br. Zeitschrift Fur Physikalische Chemie, 2013, 227, .	2.8	8
336	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.	2.8	8
337	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.	5.3	8
338	Dependence of the chemical dynamics of intercluster association reactions on the strength of the soluteâ€“solvent intermolecular potential. Journal of Chemical Physics, 1993, 98, 7826-7837.	3.0	7
339	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.	2.5	7
340	A chemical dynamics study of the HClÂ+ HCl+ reaction. International Journal of Mass Spectrometry, 2021, 462, 116515.	1.5	7
341	Energetics of methylene radicals formed by the 214-nm photolysis of diazomethane. The Journal of Physical Chemistry, 1978, 82, 1850-1855.	2.9	6
342	Effect of solvation on the dynamics of H + CH3 association. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1992, 25, 57-65.	1.0	6

#	Article	IF	Citations
343	NH₄⁺ + CH₄ Gas Phase Collisions as a Possible Analogue to Protonated Peptide/Surface Induced Dissociation. Journal of Physical Chemistry A, 2009, 113, 7543-7547.	2.5	6
344	Potential energy surface for dissociation including spinâ€“orbit effects. Molecular Physics, 2012, 110, 2599-2609.	1.7	6
345	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.	3.0	6
346	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.	2.5	6
347	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.	3.0	6
348	Sampling initial positions and momenta for nuclear trajectories from quantum mechanical distributions. Journal of Chemical Physics, 2021, 154, 074115.	3.0	6
349	Overview of Unimolecular Dynamics. , 1981, , 1-35.		6
350	Kinetic study of the reaction of methylene radicals with dimethylsilane. Decomposition of chemically activated trimethylsilane and methylethylsilane. The Journal of Physical Chemistry, 1972, 76, 459-468.	2.9	5
351	Decomposition of chemically activated ethyltrimethylgermane the arrheniusA-factors for rupture of group IVA?methyl bonds. International Journal of Chemical Kinetics, 1975, 7, 547-555.	1.6	5
352	Predissociation of chloroacetylene. Journal of Chemical Physics, 1976, 64, 2256-2257.	3.0	5
353	Gas phase ion chemistry: a fruitful playground for the interplay between experiment and theory. International Journal of Mass Spectrometry, 2000, 201, ix-x.	1.5	5
354	Role of computational chemistry in the theory of unimolecular reaction rates. , 2005, , 397-423.		5
355	Chemical Dynamics Simulations of Energy Transfer and Unimolecular Decomposition in Collision-Induced Dissociation (CID) and Surface-Induced Dissociation (SID). , 2006, , 379-432.		5
356	OÂ+ÂC2H4 potential energy surface: lowest-lying singlet at the multireference level. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	5
357	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.	3.1	5
358	PSO Method for Fitting Analytic Potential Energy Functions. Application to Iâ€“(H2O). Journal of Chemical Theory and Computation, 2018, 14, 1321-1332.	5.3	5
359	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.	2.5	5
360	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.	2.8	5

#	Article	IF	Citations
361	Dynamics of proton transfer from ArH+ to CO. International Journal of Mass Spectrometry, 2019, 438, 175-185.	1.5	5
362	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.	1.5	5
363	Collisional dynamics simulations revealing fragmentation properties of Zn(<scp>ii</scp>)-bound poly-peptide. Physical Chemistry Chemical Physics, 2020, 22, 14551-14559.	2.8	5
364	Direct Dynamics Simulations of the Thermal Fragmentation of a Protonated Peptide Containing Arginine. ACS Omega, 2020, 5, 1463-1471.	3.5	5
365	Unimolecular Fragmentation Properties of Thermometer Ions from Chemical Dynamics Simulations. Journal of the American Society for Mass Spectrometry, 2021, 32, 169-179.	2.8	5
366	Semiclassical eigenvalues of a three-dimensional Hamiltonian with one arbitrary trajectory. Chemical Physics Letters, 1985, 114, 248-252.	2.6	4
367	Anharmonic Semiclassical Variational Transition-State Theory Rate Constant Model for H Atom Association with Different Sites on the Diamond {111} Surfaceâ€. Journal of Physical Chemistry A, 2001, 105, 2453-2457.	2.5	4
368	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.	2.5	4
369	Is CH3NC isomerization an intrinsic non-RRKM unimolecular reaction?. Journal of Chemical Physics, 2019, 151, 184110.	3.0	4
370	Structures and binding energies for complexations of different spin states of Ni⁺ and Ni²⁺ to aromatic molecules. Molecular Physics, 2019, 117, 1392-1403.	1.7	4
371	Reply to Carrâ€™s comments. Journal of Chemical Physics, 1978, 68, 4329-4331.	3.0	3
372	Effect of the Arâ€“Ni(s) potential on the cross section for Ar+CH4/Ni{111} collision-induced desorption and the need for a more accurate CH4/Ni{111} potential. Journal of Chemical Physics, 2005, 122, 044704.	3.0	3
373	Representing and Selecting Vibrational Angular Momentum States for Quasiclassical Trajectory Chemical Dynamics Simulations. Journal of Physical Chemistry A, 2007, 111, 10292-10301.	2.5	3
374	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.	4.6	3
375	Addressing an instability in unrestricted density functional theory direct dynamics simulations. Journal of Computational Chemistry, 2019, 40, 933-936.	3.3	3
376	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.	2.5	3
377	Accurate Phase Space Theory and Molecular Dynamics Calculations of Aluminum Cluster Dissociation. Springer Series in Cluster Physics, 1999, , 228-254.	0.3	3
378	A Ubiquitous Tool for Education in Chemical Dynamics Simulations. Ubiquitous Learning, 2009, 1, 57-62.	0.2	3

#	Article	IF	Citations
379	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, .	1.9	3
380	Empirical potential for methyl-radical association with diamond surfaces. Physical Review B, 1997, 56, 13543-13555.	3.2	2
381	Role of the Surface Site in the Kinetics of H Atom Association with Diamond Surfaces. Journal of Physical Chemistry B, 1998, 102, 382-386.	2.6	2
382	Experiments with Parallelizing Tribology Simulations. Journal of Supercomputing, 2004, 28, 323-343.	3.6	2
383	Regular Dynamics Associated with Heat Transfer at the Interface of Model Diamond {111} Nanosurfaces. Journal of Physical Chemistry C, 2007, 111, 1754-1763.	3.1	2
384	Effect of Potential Energy Surface Properties on Unimolecular Dynamics for a Model Alkyl Radical Dissociation Reaction: H-C-C â†’ H + C=C. , 1981, , 37-73.		2
385	Photochemistry of phenylcyclopropane. Journal of Photochemistry and Photobiology, 1979, 11, 227-239.	0.6	1
386	Dissociation and IVR pathways for the CF3H(H2O)3 cluster. Journal of Cluster Science, 1990, 1, 335-354.	3.3	1
387	Simulations of Energy Transfer in the Collision-Induced Dissociation of Al6(Oh) Clusters by Rare-Gas Impact. ACS Symposium Series, 1997, , 276-290.	0.5	1
388	Size Effects on the Kinetics of Heat Transfer from a Nanoscale Diamond Particle to a Diamond Surface. Journal of Physical Chemistry C, 2008, 112, 8564-8569.	3.1	1
389	Data Reduction Through Increased Data Utilization in Chemical Dynamics Simulations. Big Data Research, 2017, 9, 57-66.	4.2	1
390	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
391	Time-Dependent Perspective for the Intramolecular Couplings of the Nâ€“H Stretches of Protonated Tryptophan. Journal of Physical Chemistry A, 2020, 124, 4062-4067.	2.5	1
392	Editorial: Application of Optimization Algorithms in Chemistry. Frontiers in Chemistry, 2020, 8, 198.	3.6	1
393	Direct Dynamics Simulations of the ³CH₂ + ³O₂ Reaction at High Temperature. Journal of Physical Chemistry A, 2021, 125, 621-627.	2.5	1
394	Efficiency of Intramolecular Vibrational Energy Redistribution in Model Systems: Chloroacetylene. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1977, 81, 207-209.	0.9	0
395	Tribute to the Research and Professional Career of Reinhard Schinke. Journal of Physical Chemistry A, 2010, 114, 9589-9590.	2.5	0
396	A Load-Balancing Force Decomposition Scheme for Parallel Simulation of Chemical Dynamics with Multiple Inter-atomic Force Models. , 2013, , .		0

#	Article	IF	Citations
397	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.	4.6	0
398	Chemical dynamics simulations of energy transfer in CH₄ and N₂ collisions. RSC Advances, 2021, 11, 16173-16178.	3.6	0
399	Mechanism and kinetics for the reaction of methyl peroxy radical with O₂. Physical Chemistry Chemical Physics, 2021, 23, 23508-23516.	2.8	0
400	Comparing Various Parallelizing Approaches for Tribology Simulations. , 2004, , 231-252.		0