

William Hase

List of Publications by Year in descending order

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docs citations

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times ranked

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#	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.	1.5	366
4	A SN2 Reaction That Avoids Its Deep Potential Energy Minimum. Science, 2002, 296, 875-878.	6.0	357
5	On non-RRKM unimolecular kinetics: Molecules in general, and CH ₃ NC in particular. Journal of Chemical Physics, 1973, 59, 4621-4632.	1.2	315
6	Imaging Nucleophilic Substitution Dynamics. Science, 2008, 319, 183-186.	6.0	307
7	Simulations of Gas-Phase Chemical Reactions: Applications to SN2 Nucleophilic Substitution. Science, 1994, 266, 998-1002.	6.0	284
8	Ab initio classical trajectories on the Born-Oppenheimer surface: Hessian-based integrators using fifth-order polynomial and rational function fits. Journal of Chemical Physics, 1999, 111, 3800-3805.	1.2	276
9	Ab initio classical trajectory study of H ₂ CO ⁺ H ₂ +CO dissociation. Chemical Physics Letters, 1994, 228, 436-442.	1.2	198
10	Variational unimolecular rate theory. Accounts of Chemical Research, 1983, 16, 258-264.	7.6	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.	1.2	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.	0.9	147
14	Theoretical and Computational Studies of Non-RRKM Unimolecular Dynamics. Journal of Physical Chemistry A, 2009, 113, 2236-2253.	1.1	146
15	Rethinking the S _N 2 reaction. Science, 2016, 352, 32-33.	6.0	146
16	DIRECT DYNAMICS SIMULATIONS OF REACTIVE SYSTEMS. , 1998, , 143-189.		143
17	Trajectory studies of SN2 nucleophilic substitution. I. Dynamics of Cl ⁻ +CH ₃ Cl reactive collisions. Journal of Chemical Physics, 1990, 93, 7962-7980.	1.2	140
18	Trajectory studies of SN2 nucleophilic substitution. II. Nonstatistical central barrier recrossing in the Cl ⁻ +CH ₃ Cl system. Journal of Chemical Physics, 1992, 96, 8275-8287.	1.2	139

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19	Ab Initio Study of the Interaction of Water with Cluster Models of the Aluminum Terminated (0001) α -Aluminum Oxide Surface. <i>Journal of Physical Chemistry B</i> , 1998, 102, 6539-6548.	1.2	139
20	A Direct Dynamics Trajectory Study of $F + CH_3OOH$ Reactive Collisions Reveals a Major Non-IRC Reaction Path. <i>Journal of the American Chemical Society</i> , 2007, 129, 9976-9985.	6.6	139
21	Chemical Dynamics Simulations of $X + CH_3Y \rightarrow XCH_3 + Y$ Gas-Phase S_N2 Nucleophilic Substitution Reactions. Nonstatistical Dynamics and Nontraditional Reaction Mechanisms. <i>Journal of Physical Chemistry A</i> , 2012, 116, 3061-3080.	1.1	139
22	On the dynamics of state selected unimolecular reactions: Chloroacetylene dissociation and predissociation. <i>Journal of Chemical Physics</i> , 1977, 66, 1523-1533.	1.2	128
23	Direct Chemical Dynamics Simulations. <i>Journal of the American Chemical Society</i> , 2017, 139, 3570-3590.	6.6	128
24	Identification of Atomic-Level Mechanisms for Gas-Phase $X + CH_3Y \rightarrow XCH_3 + Y$ S_N2 Reactions by Combined Experiments and Simulations. <i>Accounts of Chemical Research</i> , 2014, 47, 2960-2969.	7.6	127
25	Monte carlo sampling of a microcanonical ensemble of classical harmonic oscillators. <i>Chemical Physics Letters</i> , 1980, 74, 284-287.	1.2	120
26	Thermal rate constant for hydrogen atom + methyl radical. methane recombination. 3. Comparison of experiment and canonical variational transition state theory. <i>Journal of the American Chemical Society</i> , 1987, 109, 2916-2922.	6.6	119
27	Classical mechanics of intramolecular vibrational energy flow in benzene. IV. Models with reduced dimensionality. <i>Journal of Chemical Physics</i> , 1988, 89, 6723-6735.	1.2	118
28	Some Recent Advances and Remaining Questions Regarding Unimolecular Rate Theory. <i>Accounts of Chemical Research</i> , 1998, 31, 659-665.	7.6	118
29	Direct Dynamics Simulations of Collision- and Surface-Induced Dissociation of N-Protonated Glycine. Shattering Fragmentation. <i>Journal of Physical Chemistry A</i> , 2002, 106, 9983-9992.	1.1	115
30	Born-Oppenheimer Direct Dynamics Classical Trajectory Simulations. <i>Reviews in Computational Chemistry</i> , 2003, , 79-146.	1.5	108
31	Complete multidimensional analytic potential energy surface for chloride + chloroform S_N2 nucleophilic substitution. <i>The Journal of Physical Chemistry</i> , 1990, 94, 2778-2788.	2.9	107
32	$F + CH_3I \rightarrow FCH_3 + I$ Reaction Dynamics. Nontraditional Atomistic Mechanisms and Formation of a Hydrogen-Bonded Complex. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 2747-2752.	2.1	103
33	Direct Dynamics Study of the Stereomutation of Cyclopropane. <i>Journal of the American Chemical Society</i> , 1997, 119, 5251-5252.	6.6	101
34	A direct mechanism for S_N2 nucleophilic substitution enhanced by mode-selective vibrational excitation. <i>Journal of the American Chemical Society</i> , 1989, 111, 2349-2351.	6.6	99
35	Direct Dynamics Simulation of the Lifetime of Trimethylene. <i>Journal of the American Chemical Society</i> , 1996, 118, 9922-9931.	6.6	98
36	The criterion of minimum state density in unimolecular rate theory. An application to ethane dissociation. <i>Journal of Chemical Physics</i> , 1976, 64, 2442.	1.2	97

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37	Dynamics of ethyl radical decomposition. II. Applicability of classical mechanics to large-molecule unimolecular reaction dynamics. <i>Journal of Computational Chemistry</i> , 1982, 3, 335-343.	1.5	97
38	Trajectory Studies of SN2 Nucleophilic Substitution. 8. Central Barrier Dynamics for Gas Phase Cl+ CH3Cl. <i>Journal of the American Chemical Society</i> , 2001, 123, 5753-5756.	6.6	97
39	Analytic function for the atomic hydrogen + methyl .dbrarw. methane (H + CH3 .dbrarw. CH4) potential energy surface. <i>The Journal of Physical Chemistry</i> , 1984, 88, 1339-1347.	2.9	94
40	Comparison of models for calculating the RRKM unimolecular rate constant k(E, J). <i>Chemical Physics Letters</i> , 1990, 175, 117-124.	1.2	94
41	Trajectory Studies of SN2 Nucleophilic Substitution. 4. Intramolecular and Unimolecular Dynamics of the Cl---CH3Br and ClCH3---Br- Complexes. <i>Journal of the American Chemical Society</i> , 1994, 116, 9644-9651.	6.6	94
42	Indirect Dynamics in a Highly Exoergic Substitution Reaction. <i>Journal of the American Chemical Society</i> , 2013, 135, 4250-4259.	6.6	94
43	Direct chemical dynamics simulations: coupling of classical and quasiclassical trajectories with electronic structure theory. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2013, 3, 296-316.	6.2	93
44	The VENUS/NWChem software package. Tight coupling between chemical dynamics simulations and electronic structure theory. <i>Computer Physics Communications</i> , 2014, 185, 1074-1080.	3.0	93
45	Reaction Products with Internal Energy beyond the Kinematic Limit Result from Trajectories Far from the Minimum Energy Path: An Example from H + HBr at H2+ Br. <i>Journal of the American Chemical Society</i> , 2005, 127, 16368-16369.	6.6	90
46	Energy transfer in rare gas collisions with self-assembled monolayers. <i>Journal of Chemical Physics</i> , 1997, 107, 9677-9686.	1.2	88
47	Unimolecular dynamics of Cl+...CH3Cl intermolecular complexes formed by Cl+ + CH3Cl association. <i>Journal of Chemical Physics</i> , 1995, 102, 5626-5635.	1.2	86
48	Dynamics of Energy Transfer in Peptide-Surface Collisions. <i>Journal of the American Chemical Society</i> , 2002, 124, 1524-1531.	6.6	84
49	Ab Initio Direct Dynamics Study of Cyclopropyl Radical Ring-Opening. <i>Journal of the American Chemical Society</i> , 2002, 124, 3208-3209.	6.6	83
50	Non-RRKM kinetics in gas-phase SN2 nucleophilic substitution. <i>The Journal of Physical Chemistry</i> , 1990, 94, 6148-6150.	2.9	82
51	Direct Dynamics Quasiclassical Trajectory Study of the Thermal Stereomutations of Cyclopropane. <i>Journal of Physical Chemistry A</i> , 1998, 102, 3648-3658.	1.1	82
52	Ab Initio Direct Dynamics Trajectory Study of the Cl+ CH3Cl SN2 Reaction at High Reagent Translational Energy. <i>Journal of the American Chemical Society</i> , 1999, 121, 7124-7129.	6.6	81
53	Origin of the Boltzmann translational energy distribution in the scattering of hyperthermal Ne atoms off a self-assembled monolayer. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 901-910.	1.3	81
54	Trajectory Studies of SN2 Nucleophilic Substitution. 6. Translational Activation of the Cl+ CH3Cl Reaction. <i>Journal of Physical Chemistry A</i> , 1998, 102, 6208-6214.	1.1	79

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55	Trajectory studies of SN2 nucleophilic substitution. III. Dynamical stereochemistry and energy transfer pathways for the $\text{Cl}^{\cdot+}\text{CH}_3\text{Cl}$ association and direct substitution reactions. <i>Journal of Chemical Physics</i> , 1993, 98, 8626-8639.	1.2	78
56	Collisional Activation of Small Peptides. <i>Journal of Physical Chemistry A</i> , 1999, 103, 3981-3990.	1.1	78
57	Temperature Dependence of the Rate Constants and Branching Ratios for the Reactions of $\text{Cl}(\text{D}_2\text{O})_{1-3}$ with CH_3Br and Thermal Dissociation Rates for $\text{Cl}(\text{CH}_3\text{Br})$. <i>Journal of the American Chemical Society</i> , 1997, 119, 577-584.	6.6	76
58	Dynamics of ethyl radical decomposition. 3. Effect of chemical activation vs. microcanonical sampling. <i>The Journal of Physical Chemistry</i> , 1983, 87, 2754-2763.	2.9	75
59	Modification of the Duchovic-Hase-Schlegel potential energy function for $\text{H}+\text{CH}_3\text{CH}_4$. Comparison of canonical variational transition state theory, trajectory, and experimental association rate constants. <i>Journal of Chemical Physics</i> , 1991, 95, 8073-8082.	1.2	75
60	Semiempirical MNDO, AM1, and PM3 direct dynamics trajectory studies of formaldehyde unimolecular dissociation. <i>Journal of Chemical Physics</i> , 1996, 104, 7882-7894.	1.2	74
61	Classical dynamics simulations of SiMe_3^+ ion-surface scattering. <i>Journal of Chemical Physics</i> , 1997, 106, 10337-10348.	1.2	74
62	Kinetics of $\text{F}+\text{CH}_3\text{Cl}$ SN2 Nucleophilic Substitution. <i>Journal of the American Chemical Society</i> , 1997, 119, 3093-3102.	6.6	74
63	Statistical Rate Theory Calculations of the $\text{Cl}+\text{CH}_3\text{Br}$ and ClCH_3+Br Rate Constant Versus Temperature, Translational Energy, and H(D) Isotopic Substitution. <i>Journal of the American Chemical Society</i> , 1995, 117, 9347-9356.	6.6	73
64	Statistical anharmonic unimolecular rate constants for the dissociation of fluxional molecules: Application to aluminum clusters. <i>Journal of Chemical Physics</i> , 1996, 105, 7432-7447.	1.2	73
65	Direct Dynamics Simulations of the Product Channels and Atomistic Mechanisms for the $\text{OH}+\text{CH}_3$ Reaction. Comparison with Experiment. <i>Journal of Physical Chemistry A</i> , 2013, 117, 7162-7178.	1.1	73
66	Theoretical Critical Configuration for Ethane Decomposition and Methyl Radical Recombination. <i>Journal of Chemical Physics</i> , 1972, 57, 730-733.	1.2	72
67	Quasiperiodic trajectories for a multidimensional anharmonic classical Hamiltonian excited above the unimolecular threshold. <i>Journal of Chemical Physics</i> , 1980, 73, 3779-3790.	1.2	72
68	Unimolecular and intramolecular dynamics. Relationship to potential energy surface properties. <i>The Journal of Physical Chemistry</i> , 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 Monolayer. <i>Journal of Physical Chemistry A</i> , 2003, 107, 10600-10607.	1.1	71
70	Chemical Dynamics Simulations of CO_2 Scattering off a Fluorinated Self-Assembled Monolayer Surface. <i>Journal of Physical Chemistry C</i> , 2007, 111, 354-364.	1.5	71
71	Thermal rate constant for $\text{H}+\text{CH}_3\text{CH}_4$ recombination. Comparison of quasiclassical trajectory and variational transition state theory. <i>Journal of Chemical Physics</i> , 1985, 83, 3448-3453.	1.2	70
72	UV Absorption Spectrum of Alternating DNA Duplexes. Analysis of Excitonic and Charge Transfer Interactions. <i>Journal of Physical Chemistry A</i> , 2012, 116, 11151-11160.	1.1	70

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73	Comparisons of Models for Simulating Energy Transfer in Ne-Atom Collisions with an Alkyl Thiolate Self-Assembled Monolayer. <i>Journal of Physical Chemistry B</i> , 2002, 106, 8029-8037.	1.2	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. <i>Journal of the American Chemical Society</i> , 2011, 133, 8335-8343.	6.6	69
75	A Zwitterionic Carbanion Frustrated by Boranes – Dihydrogen Cleavage with Weak Lewis Acids via an Inverse-Frustrated Lewis Pair Approach. <i>Journal of the American Chemical Society</i> , 2013, 135, 16066-16069.	6.6	69
76	Translational and vibrational energy dependence of the cross section for H + C ₂ H ₄ → C ₂ H ₅ *. <i>The Journal of Physical Chemistry</i> , 1981, 85, 958-968.	2.9	68
77	Ab initio potential energy curve for CH bond dissociation in methane. <i>Chemical Physics Letters</i> , 1982, 89, 120-125.	1.2	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. <i>The Journal of Physical Chemistry</i> , 1993, 97, 311-322.	2.9	68
79	Classical trajectory calculation of the benzene overtone spectra. <i>The Journal of Physical Chemistry</i> , 1988, 92, 3217-3225.	2.9	67
80	Classical mechanics of intramolecular vibrational energy flow in benzene. V. Effect of zero-point energy motion. <i>Journal of Chemical Physics</i> , 1989, 91, 7490-7497.	1.2	67
81	The role of state specificity in unimolecular rate theory. <i>Chemical Physics</i> , 1989, 139, 1-13.	0.9	67
82	A Model Multidimensional Analytic Potential Energy Function for the Cl + CH ₃ Br → ClCH ₃ + Br- Reaction. <i>The Journal of Physical Chemistry</i> , 1994, 98, 1608-1619.	2.9	66
83	An ab Initio Study of the Transition State and Forward and Reverse Rate Constants for C ₂ H ₅ + H + C ₂ H ₄ . <i>The Journal of Physical Chemistry</i> , 1996, 100, 5354-5361.	2.9	66
84	Trajectory Studies of S _N 2 Nucleophilic Substitution. 5. Semiempirical Direct Dynamics of Cl-CH ₃ Br Unimolecular Decomposition. <i>Journal of the American Chemical Society</i> , 1996, 118, 2257-2266.	6.6	65
85	RRKM and non-RRKM behavior in chemical activation and related studies. <i>The Journal of Physical Chemistry</i> , 1984, 88, 6717-6720.	2.9	64
86	Trajectory studies of model H ₂ C=C=H dissociation. I. Random vibrational excitation. <i>Journal of Chemical Physics</i> , 1980, 72, 316-331.	1.2	63
87	Perspective: chemical dynamics simulations of non-statistical reaction dynamics. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2017, 375, 20160204.	1.6	63
88	An analytic function describing the H+C ₂ H ₄ →C ₂ H ₅ potential energy surface. <i>Journal of Chemical Physics</i> , 1978, 69, 3548-3562.	1.2	62
89	Trajectory studies of the molecular dynamics of ethyl radical decomposition. <i>Journal of Chemical Physics</i> , 1979, 71, 2911.	1.2	61
90	Analysis and extension of a model for constraining zero-point energy flow in classical trajectory simulations. <i>Journal of Chemical Physics</i> , 1994, 100, 1179-1189.	1.2	61

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91	Trajectory Studies of SN2 Nucleophilic Substitution. 7. F- + CH3Cl $\hat{\rightarrow}$ FCH3 + Cl-. Journal of Physical Chemistry A, 1998, 102, 9819-9828.	1.1	61
92	Identifying trapping desorption in gas-surface scattering. Chemical Physics Letters, 2000, 329, 84-91.	1.2	61
93	Effect of surface stiffness on the efficiency of surface-induced dissociation. Physical Chemistry Chemical Physics, 2001, 3, 2306-2314.	1.3	60
94	Molecular Dynamics Simulation of Nanoparticle Self-Assembly at a Liquid-Liquid Interface. Langmuir, 2006, 22, 6385-6390.	1.6	60
95	Protonated Urea Collision-Induced Dissociation. Comparison of Experiments and Chemical Dynamics Simulations. Journal of Physical Chemistry A, 2009, 113, 13853-13862.	1.1	60
96	Role of angular momentum in statistical unimolecular rate theory. International Reviews in Physical Chemistry, 1991, 10, 249-286.	0.9	59
97	Post-transition state dynamics for propene ozonolysis: Intramolecular and unimolecular dynamics of molozonide. Journal of Chemical Physics, 2006, 125, 014317.	1.2	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.	6.6	59
99	Imaging dynamic fingerprints of competing E2 and SN2 reactions. Nature Communications, 2017, 8, 25.	5.8	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 Clusters. Journal of Physical Chemistry A, 2000, 104, 10556-10564.	1.1	57
102	1985, 82, 123-133.	1.2	56
103	Direct dynamics study of energy transfer and collision-induced dissociation: Effects of impact energy, geometry, and reactant vibrational mode in H2CO+Ne collisions. Journal of Chemical Physics, 2003, 119, 3040-3050.	1.2	55
104	A washboard with moment of inertia model of gas-surface scattering. Journal of Chemical Physics, 2004, 120, 1031-1043.	1.2	55
105	Electronic Structure Theory Study of the F + CH3I $\hat{\rightarrow}$ FCH3 + I Potential Energy Surface. Journal of Physical Chemistry A, 2010, 114, 9635-9643.	1.1	55
106	Simulation studies of the Cl + CH3I SN2 nucleophilic substitution reaction: Comparison with ion imaging experiments. Journal of Chemical Physics, 2013, 138, 114309.	1.2	55
107	The sensitivity of IVR in benzene to bend-stretch potential energy coupling. Journal of Chemical Physics, 1986, 85, 4422-4426.	1.2	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.	1.2	53

#	ARTICLE	IF	CITATIONS
109	Reaction dynamics of temperature-variable anion water clusters studied with crossed beams and by direct dynamics. <i>Faraday Discussions</i> , 2012, 157, 41.	1.6	53
110	Chemical dynamics simulations of the monohydrated OH ⁻ (H ₂ O) + CH ₃ I reaction. Atomic-level mechanisms and comparison with experiment. <i>Journal of Chemical Physics</i> , 2015, 142, 244308.	1.2	53
111	Intramolecular vibrational energy relaxation in benzene. <i>Chemical Physics Letters</i> , 1978, 54, 73-76.	1.2	52
112	A dynamical study of the H+CH ₃ →CH ₄ recombination reaction. <i>Journal of Chemical Physics</i> , 1985, 82, 3599-3606.	1.2	52
113	Energy Transfer Dynamics in the Collision-Induced Dissociation of Al ₆ and Al ₁₃ Clusters. <i>The Journal of Physical Chemistry</i> , 1995, 99, 8147-8161.	2.9	52
114	Thresholds for the Collision-Induced Dissociation of Clusters by Rare Gas Impact. <i>The Journal of Physical Chemistry</i> , 1996, 100, 8190-8196.	2.9	52
115	Trajectory studies of model H ₂ C=C=CH ₂ dissociation. III. Details of the lifetime distribution following chemical activation. <i>Journal of Chemical Physics</i> , 1984, 80, 714-719.	1.2	51
116	Comparison of Explicit and United Atom Models for Alkane Chains Physisorbed on γ-Al ₂ O ₃ (0001). <i>Journal of Physical Chemistry B</i> , 1999, 103, 3885-3895.	1.2	51
117	Energy transfer pathways in the collisional activation of peptides. <i>International Journal of Mass Spectrometry</i> , 2000, 201, 233-244.	0.7	51
118	Dynamics of the biradical mediating vinylcyclopropane→cyclopentene rearrangement. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 304-312.	1.3	51
119	Direct dynamics study of N-protonated diglycine surface-induced dissociation. Influence of collision energy. <i>Journal of the American Society for Mass Spectrometry</i> , 2003, 14, 1402-1412.	1.2	51
120	Accelerated direct semiclassical molecular dynamics using a compact finite difference Hessian scheme. <i>Journal of Chemical Physics</i> , 2013, 138, 054116.	1.2	50
121	A comparison of classical trajectory and statistical unimolecular rate theory calculations of Al ₃ decomposition. <i>Journal of Chemical Physics</i> , 1994, 101, 8535-8553.	1.2	49
122	Quantum mechanical study of the unimolecular dissociation of HO ₂ : A rigorous test of RRKM theory. <i>Journal of Chemical Physics</i> , 1995, 102, 5867-5870.	1.2	49
123	Quasiclassical trajectory calculations for the OH(X ² Π) and OD(X ² Π)+HBr reactions: Energy partitioning and rate constants. <i>Journal of Chemical Physics</i> , 1996, 105, 9897-9911.	1.2	49
124	Dynamics of Energy Transfer in Collisions of O(3P) Atoms with a 1-Decanethiol Self-Assembled Monolayer Surface. <i>Journal of Physical Chemistry B</i> , 2006, 110, 11863-11877.	1.2	49
125	Energy Transfer, Unfolding, and Fragmentation Dynamics in Collisions of N-Protonated Octaglycine with an H-SAM Surface. <i>Journal of the American Chemical Society</i> , 2009, 131, 17185-17193.	6.6	49
126	Comparisons of classical and Wigner sampling of transition state energy levels for quasiclassical trajectory chemical dynamics simulations. <i>Journal of Chemical Physics</i> , 2010, 133, 044313.	1.2	49

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127	Sum and density of states for anharmonic polyatomic molecules. Effect of bend-stretch coupling. <i>Journal of Chemical Physics</i> , 1983, 78, 5052-5058.	1.2	48
128	Efficiency of energy transfer in protonated diglycine and dialanine SID. <i>International Journal of Mass Spectrometry</i> , 2003, 230, 57-63.	0.7	48
129	Quasiclassical dynamics simulation of the collision-induced dissociation of Cr(CO) ₆ ⁺ with Xe. <i>Journal of Chemical Physics</i> , 2005, 123, 154311.	1.2	48
130	Properties of Complexes Formed by Na ⁺ , Mg ²⁺ , and Fe ²⁺ Binding with Benzene Molecules. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9500-9511.	1.1	48
131	Reaction path Hamiltonian analysis of the dynamics for Cl ⁻ + CH ₃ Br → ClCH ₃ + Br ⁻ SN ₂ nucleophilic substitution. <i>Chemical Physics</i> , 1996, 212, 247-258.	0.9	47
132	Comparison of direct dynamics simulations with different electronic structure methods. F ⁻ + CH ₃ I with MP2 and DFT/B97-1. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 2589-2597.	1.3	47
133	Trajectory studies of model H ₂ C=CH ⁺ H+C = C dissociation. II. Angular momenta and energy partitioning and their relation to non-RRKM dynamics. <i>Journal of Chemical Physics</i> , 1981, 75, 3809-3820.	1.2	46
134	Resolution of a paradox concerning the forward and reverse rate constants for ethyl + atomic hydrogen + ethylene. <i>The Journal of Physical Chemistry</i> , 1982, 86, 3901-3904.	2.9	46
135	Trajectory studies of S _N 2 nucleophilic substitution. IX. Microscopic reaction pathways and kinetics for Cl ⁻ +CH ₃ Br. <i>Journal of Chemical Physics</i> , 2003, 118, 2688.	1.2	46
136	Gas-Phase Chemical Dynamics Simulations on the Bifurcating Pathway of the Pimaradienyl Cation Rearrangement: Role of Enzymatic Steering in Abietic Acid Biosynthesis. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1212-1222.	2.3	46
137	How a Solvent Molecule Affects Competing Elimination and Substitution Dynamics. Insight into Mechanism Evolution with Increased Solvation. <i>Journal of the American Chemical Society</i> , 2018, 140, 10995-11005.	6.6	46
138	Dynamics of Unimolecular Reactions. , 1976, , 121-169.		45
139	Direct dynamics simulations using Hessian-based predictor-corrector integration algorithms. <i>Journal of Chemical Physics</i> , 2007, 126, 044105.	1.2	45
140	Chemical Dynamics Study of Intrasurface Hydrogen-Bonding Effects in Gas-Surface Energy Exchange and Accommodation. <i>Journal of Physical Chemistry C</i> , 2008, 112, 476-490.	1.5	45
141	Dynamics of CO ₂ Scattering off a Perfluorinated Self-Assembled Monolayer. Influence of the Incident Collision Energy, Mass Effects, and Use of Different Surface Models. <i>Journal of Physical Chemistry A</i> , 2009, 113, 3850-3865.	1.1	45
142	Use of a single trajectory to study product energy partitioning in unimolecular dissociation: Mass effects for halogenated alkanes. <i>Journal of Chemical Physics</i> , 2006, 124, 064313.	1.2	44
143	Importance of shattering fragmentation in the surface-induced dissociation of protonated octaglycine. <i>Journal of the American Society for Mass Spectrometry</i> , 2009, 20, 939-948.	1.2	44
144	Evaluating the Accuracy of Hessian Approximations for Direct Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 54-64.	2.3	44

#	ARTICLE	IF	CITATIONS
145	Effect of anharmonicity on intermolecular energy transfer from highly vibrationally excited molecules. <i>The Journal of Physical Chemistry</i> , 1988, 92, 4040-4046.	2.9	43
146	Ab initiodirect dynamics trajectory simulation of C ₂ H ₅ F + C ₂ H ₄ + HF product energy partitioning. <i>Journal of Chemical Physics</i> , 2004, 121, 8831-8845.	1.2	43
147	Classical trajectory study of the unimolecular decomposition of H ₂ Cl, H ₂ H, and Cl ₂ . <i>Journal of Chemical Physics</i> , 1974, 61, 4690-4699.	1.2	42
148	A PM3-SRP + Analytic Function Potential Energy Surface Model for O(3P) Reactions with Alkanes. Application to O(3P) + Ethane. <i>Journal of Physical Chemistry A</i> , 2004, 108, 9863-9875.	1.1	42
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