Ahren W Jasper

List of Publications by Year
in descending order

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96 papers	5,528 citations	70961 41 h-index	82410 72 g-index
101 all docs	101 docs citations	101 times ranked	2892 citing authors

#	Article	IF	Citations
1	Coherent switching with decay of mixing: An improved treatment of electronic coherence for non-Bornâ€“Oppenheimer trajectories. Journal of Chemical Physics, 2004, 121, 7658.	1.2	288
2	Non-Bornâ^'Oppenheimer Molecular Dynamics. Accounts of Chemical Research, 2006, 39, 101-108.	7.6	197
3	Introductory lecture: Nonadiabatic effects in chemical dynamics. Faraday Discussions, 2004, 127, 1.	1.6	190
4	Kinetics of the Reaction of Methyl Radical with Hydroxyl Radical and Methanol Decompositionâ€. Journal of Physical Chemistry A, 2007, 111, 3932-3950.	1.1	188
5	Ab initio methods for reactive potential surfaces. Physical Chemistry Chemical Physics, 2007, 9, 4055.	1.3	158
6	Fewest-switches with time uncertainty: A modified trajectory surface-hopping algorithm with better accuracy for classically forbidden electronic transitions. Journal of Chemical Physics, 2002, 116, 5424-5431.	1.2	153
7	Non-Bornâ€“Oppenheimer trajectories with self-consistent decay of mixing. Journal of Chemical Physics, 2004, 120, 5543-5557.	1.2	150
8	The reaction between propene and hydroxyl. Physical Chemistry Chemical Physics, 2009, 11, 11040.	1.3	147
9	Lennardâ€“Jones parameters for combustion and chemical kinetics modeling from full-dimensional intermolecular potentials. Combustion and Flame, 2014, 161, 101-110.	2.8	147
10	Detection and Identification of the Keto-Hydroperoxide (HOOCH₂OCHO) and Other Intermediates during Low-Temperature Oxidation of Dimethyl Ether. Journal of Physical Chemistry A, 2015, 119, 7361-7374.	1.1	143
11	Predictive a priori pressure-dependent kinetics. Science, 2014, 346, 1212-1215.	6.0	142
12	Theoretical Unimolecular Kinetics for CH₄ + M â‡„ CH₃ + H + M in Eight Baths, M = He, Ne, Ar, Kr, H₂, N₂, CO, and CH₄. Journal of Physical Chemistry A, 2011, 115, 6438-6455.	1.1	132
13	Temperature- and pressure-dependent rate coefficients for the HACA pathways from benzene to naphthalene. Proceedings of the Combustion Institute, 2017, 36, 919-926.	2.4	115
14	Non-Born-Oppenheimer Liouville-von Neumann Dynamics. Evolution of a Subsystem Controlled by Linear and Population-Driven Decay of Mixing with Decoherent and Coherent Switching. Journal of Chemical Theory and Computation, 2005, 1, 527-540.	2.3	114
15	Improved treatment of momentum at classically forbidden electronic transitions in trajectory surface hopping calculations. Chemical Physics Letters, 2003, 369, 60-67.	1.2	106
16	Quantification of the Keto-Hydroperoxide (HOOCH₂OCHO) and Other Elusive Intermediates during Low-Temperature Oxidation of Dimethyl Ether. Journal of Physical Chemistry A, 2016, 120, 7890-7901.	1.1	104
17	Hydrogen-assisted isomerizations of fulvene to benzene and of larger cyclic aromatic hydrocarbons. Proceedings of the Combustion Institute, 2013, 34, 279-287.	2.4	99
18	â€œThird-Bodyâ€•collision efficiencies for combustion modeling: Hydrocarbons in atomic and diatomic baths. Proceedings of the Combustion Institute, 2015, 35, 197-204.	2.4	97

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19	Nitrous oxide dimer: A new potential energy surface and rovibrational spectrum of the nonpolar isomer. Journal of Chemical Physics, 2010, 133, 134304.	1.2	94
20	Roaming radicals in the thermal decomposition of dimethyl ether: Experiment and theory. Combustion and Flame, 2011, 158, 618-632.	2.8	92
21	The treatment of classically forbidden electronic transitions in semiclassical trajectory surface hopping calculations. Journal of Chemical Physics, 2001, 115, 1804-1816.	1.2	91
22	Combustion chemistry in the twenty-first century: Developing theory-informed chemical kinetics models. Progress in Energy and Combustion Science, 2021, 83, 100886.	15.8	89
23	Theoretical rate coefficients for the reaction of methyl radical with hydroperoxyl radical and for methylhydroperoxide decomposition. Proceedings of the Combustion Institute, 2009, 32, 279-286.	2.4	87
24	Collisional Energy Transfer in Unimolecular Reactions: Direct Classical Trajectories for CH₄ â‡„ CH₃ + H in Helium. Journal of Physical Chemistry A, 2009, 113, 5612-5619.	1.1	87
25	Structures, Rugged Energetic Landscapes, and Nanothermodynamics of Aln (2 â‰¤ n â‰¤ 65) Particles. Journal of the American Chemical Society, 2007, 129, 14899-14910.	6.6	85
26	Quantum Mechanical and Quasiclassical Trajectory Surface Hopping Studies of the Electronically Nonadiabatic Predissociation of the Ã f State of NaH2. Journal of Physical Chemistry A, 1999, 103, 6309-6326.	1.1	77
27	Electronic decoherence time for non-Born-Oppenheimer trajectories. Journal of Chemical Physics, 2005, 123, 064103.	1.2	77
28	Pressure-dependent rate constants for PAH growth: formation of indene and its conversion to naphthalene. Faraday Discussions, 2016, 195, 637-670.	1.6	76
29	Army ants algorithm for rare event sampling of delocalized nonadiabatic transitions by trajectory surface hopping and the estimation of sampling errors by the bootstrap method. Journal of Chemical Physics, 2004, 120, 3586-3597.	1.2	74
30	Collision Efficiency of Water in the Unimolecular Reaction CH₄ (+H₂O) â‡† CH₃ + H (+H₂O): One-Dimensional and Two-Dimensional Solutions of the Low-Pressure-Limit Master Equation. Journal of Physical Chemistry A, 2013, 117, 12243-12255.	1.1	65
31	Automated computational thermochemistry for butane oxidation: A prelude to predictive automated combustion kinetics. Proceedings of the Combustion Institute, 2019, 37, 363-371.	2.4	62
32	Thermal Dissociation and Roaming Isomerization of Nitromethane: Experiment and Theory. Journal of Physical Chemistry A, 2015, 119, 7872-7893.	1.1	59
33	Theoretical and Experimental Spectroscopy of the S₂ State of CHF and CDF: Dynamically Weighted Multireference Configuration Interaction Calculations for High-Lying Electronic States. Journal of Physical Chemistry Letters, 2010, 1, 641-646.	2.1	57
34	Theory and modeling of relevance to prompt-NO formation at high pressure. Combustion and Flame, 2018, 195, 3-17.	2.8	57
35	Non-Born-Oppenheimer molecular dynamics of Naâ‹¯FH photodissociation. Journal of Chemical Physics, 2007, 127, 194306.	1.2	55
36	Low-Temperature Oxidation of Ethylene by Ozone in a Jet-Stirred Reactor. Journal of Physical Chemistry A, 2018, 122, 8674-8685.	1.1	55

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37	Do Semiclassical Trajectory Theories Provide an Accurate Picture of Radiationless Decay for Systems with Accessible Surface Crossings?. Journal of Physical Chemistry A, 2000, 104, 217-232.	1.1	53
38	Chemical Structures of Low-Pressure Premixed Methylcyclohexane Flames as Benchmarks for the Development of a Predictive Combustion Chemistry Model. Energy & Fuels, 2011, 25, 5611-5625.	2.5	48
39	Separability of Tight and Roaming Pathways to Molecular Decomposition. Journal of Physical Chemistry A, 2012, 116, 6967-6982.	1.1	48
40	NON-BORN-OPPENHEIMER CHEMISTRY: POTENTIAL SURFACES, COUPLINGS, AND DYNAMICS. Advanced Series in Physical Chemistry, 2004, , 329-391.	1.5	47
41	Photodissociation of LiFH and NaFH van der Waals complexes: A semiclassical trajectory study. Journal of Chemical Physics, 2001, 115, 7945-7952.	1.2	46
42	On the Rate Constant for NH₂+HO₂ and Third-Body Collision Efficiencies for NH₂+H(+M) and NH₂+NH₂(+M). Journal of Physical Chemistry A, 2021, 125, 1505-1516.	1.1	43
43	First-principles binary diffusion coefficients for H, H2, and four normal alkanes + N2. Journal of Chemical Physics, 2014, 141, 124313.	1.2	42
44	Theoretical kinetics of O + C2H4. Proceedings of the Combustion Institute, 2017, 36, 219-227.	2.4	42
45	Coupled quasidiabatic potential energy surfaces for LiFH. Journal of Chemical Physics, 2002, 116, 8353.	1.2	40
46	The Effect of Spinâ^'Orbit Splitting on the Association Kinetics of Barrierless Halogen Atomâ^'Hydrocarbon Radical Reactions. Journal of Physical Chemistry A, 2010, 114, 5759-5768.	1.1	40
47	Identification of Tetrahydrofuran Reaction Pathways in Premixed Flames. Zeitschrift Fur Physikalische Chemie, 2011, 225, 1237-1270.	1.4	38
48	The vibrationâ€“rotationâ€“tunneling spectrum of the polar and T-shaped-N-in isomers of (NNO)2. Journal of Molecular Spectroscopy, 2011, 268, 53-65.	0.4	38
49	Conical intersections and semiclassical trajectories: Comparison to accurate quantum dynamics and analyses of the trajectories. Journal of Chemical Physics, 2005, 122, 044101.	1.2	37
50	Analytic Potential Energy Functions for Simulating Aluminum Nanoparticles. Journal of Physical Chemistry B, 2005, 109, 3915-3920.	1.2	36
51	Nascent energy distribution of the Criegee intermediate CH2OO from direct dynamics calculations of primary ozonide dissociation. Journal of Chemical Physics, 2018, 148, 174306.	1.2	36
52	Kinetics of Propargyl Radical Dissociation. Journal of Physical Chemistry A, 2015, 119, 7780-7791.	1.1	35
53	Critical Properties of Aluminum. Journal of the American Chemical Society, 2006, 128, 4224-4225.	6.6	34
54	Coupled-surface investigation of the photodissociation of NH3(Aìf): Effect of exciting the symmetric and antisymmetric stretching modes. Journal of Chemical Physics, 2009, 130, 234303.	1.2	34

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55	The Dissociation of Diacetyl: A Shock Tube and Theoretical Study. Journal of Physical Chemistry A, 2009, 113, 8318-8326.	1.1	34
56	Global potential energy surface, vibrational spectrum, and reaction dynamics of the first excited (Aìƒâ€‰A2â€²) state of HO2. Journal of Chemical Physics, 2010, 133, 144306.	1.2	34
57	Multidimensional Effects in Nonadiabatic Statistical Theories of Spin-Forbidden Kinetics: A Case Study of ³O + CO â†' CO₂. Journal of Physical Chemistry A, 2015, 119, 7339-7351.	1.1	33
58	Exploring the negative temperature coefficient behavior of acetaldehyde based on detailed intermediate measurements in a jet-stirred reactor. Combustion and Flame, 2018, 192, 120-129.	2.8	31
59	Watching a hydroperoxyalkyl radical (â€¢QOOH) dissociate. Science, 2021, 373, 679-682.	6.0	31
60	Adiabatic States Derived from a Spin-Coupled Diabatic Transformation: Semiclassical Trajectory Study of Photodissociation of HBr and the Construction of Potential Curves for LiBr⁺. Journal of Physical Chemistry A, 2008, 112, 5756-5769.	1.1	30
61	Comment on â€œWhen Rate Constants Are Not Enoughâ€• Journal of Physical Chemistry A, 2016, 120, 306-312.	1.1	30
62	Identification of the Criegee intermediate reaction network in ethylene ozonolysis: impact on energy conversion strategies and atmospheric chemistry. Physical Chemistry Chemical Physics, 2019, 21, 7341-7357.	1.3	29
63	Microcanonical Rate Constants for Unimolecular Reactions in the Low-Pressure Limit. Journal of Physical Chemistry A, 2020, 124, 1205-1226.	1.1	29
64	Secondary Kinetics of Methanol Decomposition:â€‰ Theoretical Rate Coefficients for ³CH₂ + OH, ³CH₂ + ³CH₂, and ³CH₂ + CH₃. Journal of Physical Chemistry A, 2007, 111, 8699-8707.	1.1	26
65	Non-Bornâ€“Oppenheimer molecular dynamics of the spin-forbidden reaction O(3P) + CO(Xâ€‰1Î£+) â†' CO2($ilde X{}^1Sigma _g^ +$XìƒÎ£g+1). Journal of Chemical Physics, 2013, 139, 154313.	1.2	26
66	Narrow Subthreshold Quantum Mechanical Resonances in the Li + HF â†' H + LiF Reaction. Journal of Physical Chemistry A, 2003, 107, 7236-7247.	1.1	24
67	Analytic Potential Energy Functions for Aluminum Clusters. Journal of Physical Chemistry B, 2004, 108, 8996-9010.	1.2	24
68	Isomer-Selective Detection of Keto-Hydroperoxides in the Low-Temperature Oxidation of Tetrahydrofuran. Journal of Physical Chemistry A, 2019, 123, 8274-8284.	1.1	24
69	â€œThirdâ€•bodyâ€•collision parameters for hydrocarbons, alcohols, and hydroperoxides and an effective internal rotor approach for estimating them. International Journal of Chemical Kinetics, 2020, 52, 387-402.	1.0	23
70	Anharmonic state counts and partition functions for molecules via classical phase space integrals in curvilinear coordinates. Journal of Chemical Physics, 2013, 138, 194109.	1.2	22
71	Nonthermal rate constants for CH4* + X â†' CH3 + HX, X = H, O, OH, and O2. Journal of Chemical Physics, 2019, 150, 114112.	1.2	21
72	Parameterization Strategies for Intermolecular Potentials for Predicting Trajectory-Based Collision Parameters. Journal of Physical Chemistry A, 2019, 123, 3464-3480.	1.1	19

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73	A reaction mechanism for ozone dissociation and reaction with hydrogen at elevated temperature. Fuel, 2022, 322, 124138.	3.4	19
74	Recombination and dissociation of 2-methyl allyl radicals: Experiment and theory. Proceedings of the Combustion Institute, 2017, 36, 211-218.	2.4	17
75	Anharmonic Rovibrational Partition Functions at High Temperatures: Tests of Reduced-Dimensional Models for Systems with up to Three Fluxional Modes. Journal of Physical Chemistry A, 2019, 123, 6210-6228.	1.1	16
76	An experimental and theoretical study of the high temperature reactions of the four butyl radical isomers. Physical Chemistry Chemical Physics, 2020, 22, 18304-18319.	1.3	16
77	Low- and intermediate-temperature oxidation of dimethyl ether up to 100 atm in a supercritical pressure jet-stirred reactor. Combustion and Flame, 2022, 243, 112059.	2.8	16
78	Phase Behavior of Elemental Aluminum Using Monte Carlo Simulations. Journal of Physical Chemistry B, 2006, 110, 26135-26142.	1.2	15
79	Anharmonic Rovibrational Partition Functions for Fluxional Species at High Temperatures via Monte Carlo Phase Space Integrals. Journal of Physical Chemistry A, 2018, 122, 1727-1740.	1.1	15
80	Cool flame chemistry of diesel surrogate compounds: n-Decane, 2-methylnonane, 2,7-dimethyloctane, and n-butylcyclohexane. Combustion and Flame, 2020, 219, 384-392.	2.8	15
81	Termolecular chemistry facilitated by radical-radical recombinations and its impact on flame speed predictions. Proceedings of the Combustion Institute, 2021, 38, 515-522.	2.4	15
82	Large Intermediates in Hydrazine Decomposition: A Theoretical Study of the N₃H₅ and N₄H₆ Potential Energy Surfaces. Journal of Physical Chemistry A, 2019, 123, 4679-4692.	1.1	14
83	Permutationally Invariant Polynomial Expansions with Unrestricted Complexity. Journal of Chemical Theory and Computation, 2021, 17, 5440-5455.	2.3	14
84	Extreme Low-Temperature Combustion Chemistry: Ozone-Initiated Oxidation of Methyl Hexanoate. Journal of Physical Chemistry A, 2020, 124, 9897-9914.	1.1	13
85	Anharmonic Vibrational Properties from Intrinsic n-Mode State Densities. Journal of Physical Chemistry Letters, 2013, 4, 2430-2435.	2.1	10
86	Toward accurate high temperature anharmonic partition functions. Proceedings of the Combustion Institute, 2019, 37, 315-322.	2.4	10
87	Identification of the acetaldehyde oxide Criegee intermediate reaction network in the ozone-assisted low-temperature oxidation of trans-2-butene. Physical Chemistry Chemical Physics, 2021, 23, 23554-23566.	1.3	10
88	The Role of Excited Electronic States in Hypervelocity Collisions: Enhancement of the O(³P) + HCl â†' OCl + H Reaction Channel. Journal of Physical Chemistry Letters, 2010, 1, 2940-2945.	2.1	9
89	The impact of the third O2 addition reaction network on ignition delay times of neo-pentane. Proceedings of the Combustion Institute, 2021, 38, 299-307.	2.4	8
90	Determination of the collisional energy transfer distribution responsible for the collision-induced dissociation of NO2 with Ar. Chemical Physics Letters, 2015, 636, 1-14.	1.2	7

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91	Predicting third-body collision efficiencies for water and other polyatomic baths. Faraday Discussions, 0, 238, 68-86.	1.6	7
92	Transferability of Orthogonal and Nonorthogonal Tight-Binding Models for Aluminum Clusters and Nanoparticles. Journal of Chemical Theory and Computation, 2007, 3, 210-218.	2.3	6
93	Theoretical investigation of intersystem crossing in the cyanonitrene molecule, 1NCN â†'â€ˆ3NCN. Journal of Chemical Physics, 2017, 147, 084310.	1.2	6
94	Ab initio Variational Transition State Theory and Master Equation Study of the Reaction (OH)₃SiOCH₂â€¯+â€¯CH₃â€¯â‡Œâ€¯(OH)₃SiOC₂H₅. Zeitschrift Fur Physikalische Chemie, 2015, 229, 691-708.	1.4	5
95	Parsimonious Potential Energy Surface Expansions Using Dictionary Learning with Multipass Greedy Selection. Journal of Physical Chemistry Letters, 2021, 12, 9169-9174.	2.1	5
96	Theoretical Study of the Tiâ€“Cl Bond Cleavage Reaction in TiCl₄. Zeitschrift Fur Physikalische Chemie, 2017, 231, 1489-1506.	1.4	4