Ahren W Jasper

List of Publications by Citations

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96 papers	4,444 citations	39 h-index	64 g-index
101 ext. papers	5,072 ext. citations	5.2 avg, IF	5.93 L-index

#	Paper	IF	Citations
96	Coherent switching with decay of mixing: an improved treatment of electronic coherence for non-Born-Oppenheimer trajectories. *Journal of Chemical Physics*, **2004**, 121, 7658-70	3.9	247
95	Non-Born-Oppenheimer molecular dynamics. *Accounts of Chemical Research*, **2006**, 39, 101-8	24.3	173
94	Introductory lecture: nonadiabatic effects in chemical dynamics. *Faraday Discussions*, **2004**, 127, 1-22	3.6	167
93	Kinetics of the reaction of methyl radical with hydroxyl radical and methanol decomposition. *Journal of Physical Chemistry A*, **2007**, 111, 3932-50	2.8	164
92	Ab initio methods for reactive potential surfaces. *Physical Chemistry Chemical Physics*, **2007**, 9, 4055-70	3.6	145
91	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	3.9	132
90	Non-Born-Oppenheimer trajectories with self-consistent decay of mixing. *Journal of Chemical Physics*, **2004**, 120, 5543-57	3.9	131
89	The reaction between propene and hydroxyl. *Physical Chemistry Chemical Physics*, **2009**, 11, 11040-53	3.6	121
88	Theoretical unimolecular kinetics for CH4 + M ? CH3 + H + M in eight baths, M = He, Ne, Ar, Kr, H2, N2, CO, and CH4. *Journal of Physical Chemistry A*, **2011**, 115, 6438-55	2.8	118
87	Predictive a priori pressure-dependent kinetics. *Science*, **2014**, 346, 1212-5	33.3	115
86	Lennard□ones parameters for combustion and chemical kinetics modeling from full-dimensional intermolecular potentials. *Combustion and Flame*, **2014**, 161, 101-110	5.3	112
85	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, 7361-74	2.8	111
84	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, 527-40	6.4	94
83	Nitrous oxide dimer: a new potential energy surface and rovibrational spectrum of the nonpolar isomer. *Journal of Chemical Physics*, **2010**, 133, 134304	3.9	87
82	Hydrogen-assisted isomerizations of fulvene to benzene and of larger cyclic aromatic hydrocarbons. *Proceedings of the Combustion Institute*, **2013**, 34, 279-287	5.9	84
81	Temperature- and pressure-dependent rate coefficients for the HACA pathways from benzene to naphthalene. *Proceedings of the Combustion Institute*, **2017**, 36, 919-926	5.9	83
80	Structures, rugged energetic landscapes, and nanothermodynamics of Al(n) (2 . *Journal of the American Chemical Society*, **2007**, 129, 14899-910	16.4	81

79	The treatment of classically forbidden electronic transitions in semiclassical trajectory surface hopping calculations. *Journal of Chemical Physics*, **2001**, 115, 1804-1816	3.9	81
78	Third-Body Collision efficiencies for combustion modeling: Hydrocarbons in atomic and diatomic baths. *Proceedings of the Combustion Institute*, **2015**, 35, 197-204	5.9	80
77	Improved treatment of momentum at classically forbidden electronic transitions in trajectory surface hopping calculations. *Chemical Physics Letters*, **2003**, 369, 60-67	2.5	80
76	Roaming radicals in the thermal decomposition of dimethyl ether: Experiment and theory. *Combustion and Flame*, **2011**, 158, 618-632	5.3	79
75	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	5.9	77
74	Collisional energy transfer in unimolecular reactions: direct classical trajectories for CH4 CH3 + H in helium. *Journal of Physical Chemistry A*, **2009**, 113, 5612-9	2.8	77
73	Quantification of the Keto-Hydroperoxide (HOOCHOCHO) and Other Elusive Intermediates during Low-Temperature Oxidation of Dimethyl Ether. *Journal of Physical Chemistry A*, **2016**, 120, 7890-7901	2.8	72
72	Quantum Mechanical and Quasiclassical Trajectory Surface Hopping Studies of the Electronically Nonadiabatic Predissociation of the State of NaH2. *Journal of Physical Chemistry A*, **1999**, 103, 6309-6326	2.8	71
71	Electronic decoherence time for non-Born-Oppenheimer trajectories. *Journal of Chemical Physics*, **2005**, 123, 64103	3.9	67
70	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, 3586-97	3.9	63
69	Collision efficiency of water in the unimolecular reaction CH4 (+H2O) ? CH3 + H (+H2O): one-dimensional and two-dimensional solutions of the low-pressure-limit master equation. *Journal of Physical Chemistry A*, **2013**, 117, 12243-55	2.8	59
68	Pressure-dependent rate constants for PAH growth: formation of indene and its conversion to naphthalene. *Faraday Discussions*, **2016**, 195, 637-670	3.6	58
67	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	6.4	52
66	Thermal Dissociation and Roaming Isomerization of Nitromethane: Experiment and Theory. *Journal of Physical Chemistry A*, **2015**, 119, 7872-93	2.8	51
65	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	2.8	47
64	Separability of tight and roaming pathways to molecular decomposition. *Journal of Physical Chemistry A*, **2012**, 116, 6967-82	2.8	44
63	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	4.1	42
62	Non-Born-Oppenheimer molecular dynamics of Na...FH photodissociation. *Journal of Chemical Physics*, **2007**, 127, 194306	3.9	42

61	NON-BORN-OPPENHEIMER CHEMISTRY: POTENTIAL SURFACES, COUPLINGS, AND DYNAMICS. *Advanced Series in Physical Chemistry*, **2004**, 329-391		42
60	Coupled quasidiabatic potential energy surfaces for LiFH. *Journal of Chemical Physics*, **2002**, 116, 8353	3.9	40
59	The effect of spin-orbit splitting on the association kinetics of barrierless halogen atom-hydrocarbon radical reactions. *Journal of Physical Chemistry A*, **2010**, 114, 5759-68	2.8	39
58	Photodissociation of LiFH and NaFH van der Waals complexes: A semiclassical trajectory study. *Journal of Chemical Physics*, **2001**, 115, 7945-7952	3.9	39
57	Automated computational thermochemistry for butane oxidation: A prelude to predictive automated combustion kinetics. *Proceedings of the Combustion Institute*, **2019**, 37, 363-371	5.9	37
56	Identification of Tetrahydrofuran Reaction Pathways in Premixed Flames. *Zeitschrift Fur Physikalische Chemie*, **2011**, 225, 1237-1270	3.1	35
55	The vibration□otation□unneling spectrum of the polar and T-shaped-N-in isomers of (NNO)2. *Journal of Molecular Spectroscopy*, **2011**, 268, 53-65	1.3	35
54	Analytic potential energy functions for simulating aluminum nanoparticles. *Journal of Physical Chemistry B*, **2005**, 109, 3915-20	3.4	35
53	Conical intersections and semiclassical trajectories: comparison to accurate quantum dynamics and analyses of the trajectories. *Journal of Chemical Physics*, **2005**, 122, 44101	3.9	34
52	Critical properties of aluminum. *Journal of the American Chemical Society*, **2006**, 128, 4224-5	16.4	34
51	Theoretical kinetics of O + C2H4. *Proceedings of the Combustion Institute*, **2017**, 36, 219-227	5.9	32
50	Coupled-surface investigation of the photodissociation of NH3(A): effect of exciting the symmetric and antisymmetric stretching modes. *Journal of Chemical Physics*, **2009**, 130, 234303	3.9	32
49	Theory and modeling of relevance to prompt-NO formation at high pressure. *Combustion and Flame* , **2018**, 195, 3-17	5.3	32
48	The dissociation of diacetyl: a shock tube and theoretical study. *Journal of Physical Chemistry A*, **2009**, 113, 8318-26	2.8	31
47	Combustion chemistry in the twenty-first century: Developing theory-informed chemical kinetics models. *Progress in Energy and Combustion Science*, **2021**, 83, 100886	33.6	31
46	Global potential energy surface, vibrational spectrum, and reaction dynamics of the first excited (□□(2)A(')) state of HO(2). *Journal of Chemical Physics*, **2010**, 133, 144306	3.9	30
45	Low-Temperature Oxidation of Ethylene by Ozone in a Jet-Stirred Reactor. *Journal of Physical Chemistry A*, **2018**, 122, 8674-8685	2.8	30
44	First-principles binary diffusion coefficients for H, H□and four normal alkanes + N□*Journal of Chemical Physics*, **2014**, 141, 124313	3.9	29

43	Multidimensional Effects in Nonadiabatic Statistical Theories of Spin-Forbidden Kinetics: A Case Study of (3)O + CO -o CO2. *Journal of Physical Chemistry A*, **2015**, 119, 7339-51	2.8	28
42	Kinetics of Propargyl Radical Dissociation. *Journal of Physical Chemistry A*, **2015**, 119, 7780-91	2.8	27
41	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, 5756-69	2.8	27
40	Non-Born-Oppenheimer molecular dynamics of the spin-forbidden reaction O(3P) + CO(X(1)Σ) -o CO2(X (1)Σ(+)). *Journal of Chemical Physics*, **2013**, 139, 154313	3.9	24
39	Narrow Subthreshold Quantum Mechanical Resonances in the Li + HF -o H + LiF Reaction. *Journal of Physical Chemistry A*, **2003**, 107, 7236-7247	2.8	24
38	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	5.3	23
37	Comment on "When Rate Constants Are Not Enough". *Journal of Physical Chemistry A*, **2016**, 120, 306-12	2.8	23
36	Analytic Potential Energy Functions for Aluminum Clusters. *Journal of Physical Chemistry B*, **2004**, 108, 8996-9010	3.4	23
35	Secondary kinetics of methanol decomposition: theoretical rate coefficients for 3CH2 + OH, 3CH2 + 3CH2, and 3CH2 + CH3. *Journal of Physical Chemistry A*, **2007**, 111, 8699-707	2.8	21
34	Anharmonic state counts and partition functions for molecules via classical phase space integrals in curvilinear coordinates. *Journal of Chemical Physics*, **2013**, 138, 194109	3.9	20
33	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	3.6	19
32	Microcanonical Rate Constants for Unimolecular Reactions in the Low-Pressure Limit. *Journal of Physical Chemistry A*, **2020**, 124, 1205-1226	2.8	17
31	Nascent energy distribution of the Criegee intermediate CHOO from direct dynamics calculations of primary ozonide dissociation. *Journal of Chemical Physics*, **2018**, 148, 174306	3.9	17
30	Phase behavior of elemental aluminum using monte carlo simulations. *Journal of Physical Chemistry B*, **2006**, 110, 26135-42	3.4	15
29	Isomer-Selective Detection of Keto-Hydroperoxides in the Low-Temperature Oxidation of Tetrahydrofuran. *Journal of Physical Chemistry A*, **2019**, 123, 8274-8284	2.8	13
28	Nonthermal rate constants for CH + X -o CH + HX, X = H, O, OH, and O. *Journal of Chemical Physics*, **2019**, 150, 114112	3.9	13
27	On the Rate Constant for NH+HO and Third-Body Collision Efficiencies for NH+H(+M) and NH+NH(+M). *Journal of Physical Chemistry A*, **2021**, 125, 1505-1516	2.8	13
26	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	2.8	11

25	Recombination and dissociation of 2-methyl allyl radicals: Experiment and theory. *Proceedings of the Combustion Institute*, **2017**, 36, 211-218	5.9	11
24	An experimental and theoretical study of the high temperature reactions of the four butyl radical isomers. *Physical Chemistry Chemical Physics*, **2020**, 22, 18304-18319	3.6	11
23	Third-body 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	1.4	11
22	Parameterization Strategies for Intermolecular Potentials for Predicting Trajectory-Based Collision Parameters. *Journal of Physical Chemistry A*, **2019**, 123, 3464-3480	2.8	10
21	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	2.8	10
20	Anharmonic Vibrational Properties from Intrinsic n-Mode State Densities. *Journal of Physical Chemistry Letters*, **2013**, 4, 2430-2435	6.4	10
19	Toward accurate high temperature anharmonic partition functions. *Proceedings of the Combustion Institute*, **2019**, 37, 315-322	5.9	9
18	The Role of Excited Electronic States in Hypervelocity Collisions: Enhancement of the O(3P) + HCl -o OCl + H Reaction Channel. *Journal of Physical Chemistry Letters*, **2010**, 1, 2940-2945	6.4	9
17	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	5.9	7
16	Determination of the collisional energy transfer distribution responsible for the collision-induced dissociation of NO2 with Ar. *Chemical Physics Letters*, **2015**, 636, 1-14	2.5	6
15	Transferability of Orthogonal and Nonorthogonal Tight-Binding Models for Aluminum Clusters and Nanoparticles. *Journal of Chemical Theory and Computation*, **2007**, 3, 210-8	6.4	6
14	Watching a hydroperoxyalkyl radical (QOOH) dissociate. *Science*, **2021**, 373, 679-682	33.3	6
13	Permutationally Invariant Polynomial Expansions with Unrestricted Complexity. *Journal of Chemical Theory and Computation*, **2021**, 17, 5440-5455	6.4	6
12	Theoretical investigation of intersystem crossing in the cyanonitrene molecule, NCN -o NCN. *Journal of Chemical Physics*, **2017**, 147, 084310	3.9	5
11	Ab initio Variational Transition State Theory and Master Equation Study of the Reaction (OH)3SiOCH2 + CH3 ? (OH)3SiOC2H5. *Zeitschrift Fur Physikalische Chemie*, **2015**, 229, 691-708	3.1	5
10	Cool flame chemistry of diesel surrogate compounds: n-Decane, 2-methylnonane, 2,7-dimethyloctane, and n-butylcyclohexane. *Combustion and Flame*, **2020**, 219, 384-392	5.3	5
9	Large Intermediates in Hydrazine Decomposition: A Theoretical Study of the NH and NH Potential Energy Surfaces. *Journal of Physical Chemistry A*, **2019**, 123, 4679-4692	2.8	4
8	Theoretical Study of the TiCl Bond Cleavage Reaction in TiCl4. *Zeitschrift Fur Physikalische Chemie*, **2017**, 231, 1489-1506	3.1	3

List of Publications

7	Extreme Low-Temperature Combustion Chemistry: Ozone-Initiated Oxidation of Methyl Hexanoate. *Journal of Physical Chemistry A*, **2020**, 124, 9897-9914	2.8	3
6	Termolecular chemistry facilitated by radical-radical recombinations and its impact on flame speed predictions. *Proceedings of the Combustion Institute*, **2021**, 38, 515-522	5.9	3
5	Low- and intermediate-temperature oxidation of dimethyl ether up to 100 atm in a supercritical pressure jet-stirred reactor. *Combustion and Flame*, **2022**, 112059	5.3	3
4	Parsimonious Potential Energy Surface Expansions Using Dictionary Learning with Multipass Greedy Selection. *Journal of Physical Chemistry Letters*, **2021**, 12, 9169-9174	6.4	2
3	Identification of the acetaldehyde oxide Criegee intermediate reaction network in the ozone-assisted low-temperature oxidation of -2-butene. *Physical Chemistry Chemical Physics*, **2021**, 23, 23554-23566	3.6	1
2	A reaction mechanism for ozone dissociation and reaction with hydrogen at elevated temperature. *Fuel*, **2022**, 322, 124138	7.1	0
1	Aluminum Nanoparticles: Accurate Potential Energy Functions and Physical Properties169-188		