Lawrence B Harding

List of Publications by Year
in descending order

112 papers	7,381 citations	36203 51 h-index	56606 83 g-index
112 all docs	112 docs citations	112 times ranked	3745 citing authors

#	Article	IF	Citations
1	On the Enthalpy of Formation of Hydroxyl Radical and Gas-Phase Bond Dissociation Energies of Water and Hydroxyl. Journal of Physical Chemistry A, 2002, 106, 2727-2747.	1.1	466
2	The role of NNH in NO formation and control. Combustion and Flame, 2011, 158, 774-789.	2.8	304
3	Ab initio calculations of electronic and vibrational energies of HCO and HOC. Journal of Chemical Physics, 1986, 85, 911-921.	1.2	216
4	Predictive theory for the combination kinetics of two alkyl radicals. Physical Chemistry Chemical Physics, 2006, 8, 1133.	1.3	202
5	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
6	Vibrational energy levels of formaldehyde. Journal of Chemical Physics, 1985, 82, 4155-4165.	1.2	187
7	State-to-state chemistry with fast hydrogen atoms. Reaction and collisional excitation in H + CO2. Faraday Discussions of the Chemical Society, 1987, 84, 359.	2.2	180
8	Predictive Theory for Hydrogen Atomâ^'Hydrocarbon Radical Association Kinetics. Journal of Physical Chemistry A, 2005, 109, 4646-4656.	1.1	176
9	A global H2O potential energy surface for the reaction O(1D)+H2â†'OH+H. Journal of Chemical Physics, 1996, 105, 10472-10486.	1.2	175
10	Evidence for a Lower Enthalpy of Formation of Hydroxyl Radical and a Lower Gas-Phase Bond Dissociation Energy of Water. Journal of Physical Chemistry A, 2001, 105, 1-4.	1.1	175
11	Mechanisms of gas-phase and liquid-phase ozonolysis. Journal of the American Chemical Society, 1978, 100, 7180-7188.	6.6	162
12	Ab initio methods for reactive potential surfaces. Physical Chemistry Chemical Physics, 2007, 9, 4055.	1.3	158
13	Ab Initio Computations and Active Thermochemical Tables Hand in Hand: Heats of Formation of Core Combustion Species. Journal of Physical Chemistry A, 2017, 121, 6580-6602.	1.1	144
14	Predictive a priori pressure-dependent kinetics. Science, 2014, 346, 1212-1215.	6.0	142
15	A Global ab Initio Potential Energy Surface for Formaldehydeâ€. Journal of Physical Chemistry A, 2004, 108, 8980-8986.	1.1	135
16	A global A-state potential surface for H2O: Influence of excited states on the O(1D)+H2 reaction. Journal of Chemical Physics, 1997, 107, 2340-2350.	1.2	130
17	Potential energy surface and quasiclassical trajectory studies of the N(2D)+H2 reaction. Journal of Chemical Physics, 1999, 110, 9091-9100.	1.2	125
18	Roaming Radical Kinetics in the Decomposition of Acetaldehyde. Journal of Physical Chemistry A, 2010, 114, 765-777.	1.1	125

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19	The mechanism of the ene reaction of singlet oxygen with olefins. Journal of the American Chemical Society, 1980, 102, 439-449.	6.6	119
20	On the Combination Reactions of Hydrogen Atoms with Resonance-Stabilized Hydrocarbon Radicalsâ€. Journal of Physical Chemistry A, 2007, 111, 3789-3801.	1.1	111
21	Polyatomic, anharmonic, vibrational-rotational analysis. Application to accurateab initio results for formaldehyde. Journal of Computational Chemistry, 1985, 6, 13-27.	1.5	103
22	Potential energy surface and quasiclassical trajectory studies of the CN+H2 reaction. Journal of Chemical Physics, 1996, 105, 558-571.	1.2	100
23	Exploring the OH+CO reaction coordinate via infrared spectroscopy of the OHâ€“CO reactant complex. Journal of Chemical Physics, 2000, 113, 9889-9892.	1.2	97
24	The electronic states of Si2 and Siâ¯2 as revealed by photoelectron spectroscopy. Journal of Chemical Physics, 1987, 87, 5116-5124.	1.2	96
25	A quasiclassical trajectory study of the reaction OH+COâ†'H+CO2. Journal of Chemical Physics, 2003, 119, 5848-5859.	1.2	92
26	Ab initio studies of (1,2)-hydrogen migrations in open-shell hydrocarbons: vinyl radical, ethyl radical, and triplet methylcarbene. Journal of the American Chemical Society, 1981, 103, 7469-7475.	6.6	89
27	Temperature and Pressure-Dependent Rate Coefficients for the Reaction of Vinyl Radical with Molecular Oxygen. Journal of Physical Chemistry A, 2015, 119, 7766-7779.	1.1	88
28	Theoretical and Experimental Investigation of the Dynamics of the Production of CO from the CH3 + O and CD3 + O Reactions. Journal of Physical Chemistry A, 2001, 105, 8361-8369.	1.1	87
29	Reactions between Resonance-Stabilized Radicals: Propargyl + Allyl. Journal of Physical Chemistry A, 2010, 114, 4881-4890.	1.1	84
30	Methylene: ab initio vibronic analysis and reinterpretation of the spectroscopic and negative ion photoelectron experiments. Chemical Physics Letters, 1978, 55, 217-220.	1.2	79
31	A Direct Transition State Theory Based Study of Methyl Radical Recombination Kinetics. Journal of Physical Chemistry A, 1999, 103, 9388-9398.	1.1	77
32	Theoretical studies of the hydrogen peroxide potential surface. 1. An ab initio anharmonic force field. The Journal of Physical Chemistry, 1989, 93, 8004-8013.	2.9	76
33	Statistical Theory for the Kinetics and Dynamics of Roaming Reactions. Journal of Physical Chemistry A, 2011, 115, 14370-14381.	1.1	76
34	Proton transfers in hydrogen-bonded systems. 2. Electron correlation effects in diamminehydrogen(1+). Journal of the American Chemical Society, 1981, 103, 2169-2173.	6.6	75
35	Potential Energy Surface of the Ãƒ State of NH2 and the Role of Excited States in the N(2D) + H2 Reaction. Journal of Physical Chemistry A, 2000, 104, 2301-2307.	1.1	74
36	Roaming Radical Pathways for the Decomposition of Alkanes. Journal of Physical Chemistry Letters, 2010, 1, 3016-3020.	2.1	73

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37	Quantum dynamics of Rennerâ€“Teller vibronic coupling: The predissociation of HCO. Journal of Chemical Physics, 1993, 99, 5812-5827.	1.2	69
38	Mapping the OH+COâ†'HOCO reaction pathway through IR spectroscopy of the OHâ€“CO reactant complex. Faraday Discussions, 2001, 118, 373-385.	1.6	68
39	Coupled channel calculation of resonances in H+CO. Journal of Chemical Physics, 1986, 84, 4888-4893.	1.2	67
40	Theoretical Validation of Chemical Kinetic Mechanisms: Combustion of Methanol. Journal of Physical Chemistry A, 2010, 114, 8286-8301.	1.1	66
41	Theoretical studies of the low-lying states of vinylidene. Journal of the American Chemical Society, 1977, 99, 2919-2925.	6.6	64
42	Abinitiostudies on the singletâ€“triplet splitting of methylene (CH2). Journal of Chemical Physics, 1977, 67, 1777-1779.	1.2	63
43	Intermediates in the chemiluminescent reaction of singlet oxygen with ethylene. Ab initio studies. Journal of the American Chemical Society, 1977, 99, 4520-4523.	6.6	63
44	Experimental and Theoretical Investigation of the Self-Reaction of Phenyl Radicals. Journal of Physical Chemistry A, 2010, 114, 8240-8261.	1.1	63
45	Implementation of a fast analytic ground state potential energy surface for the N(2D)+H2 reaction. Journal of Chemical Physics, 2003, 119, 3063-3070.	1.2	62
46	Kinetics of CH + N₂ Revisited with Multireference Methods. Journal of Physical Chemistry A, 2008, 112, 522-532.	1.1	62
47	Ab initio theoretical studies of the Rydberg states of formaldehyde. Journal of the American Chemical Society, 1977, 99, 677-683.	6.6	60
48	Near-threshold H/D exchange in CD3CHO photodissociation. Nature Chemistry, 2011, 3, 443-448.	6.6	60
49	Thermal Dissociation and Roaming Isomerization of Nitromethane: Experiment and Theory. Journal of Physical Chemistry A, 2015, 119, 7872-7893.	1.1	59
50	A quasiclassical trajectory study of OH rotational excitation in OH+CO collisions using ab initio potential surfaces. Journal of Chemical Physics, 1992, 96, 7465-7473.	1.2	57
51	Triplet states of the amide group. Trapped electron spectra of formamide and related molecules. Chemical Physics Letters, 1975, 36, 589-593.	1.2	53
52	Theoretical studies of the hydrogen peroxide potential surface. 2. An ab initio, long-range, hydroxyl(2.PI.) + hydroxyl(2.PI.) potential. The Journal of Physical Chemistry, 1991, 95, 8653-8660.	2.9	50
53	The formaldehyde decomposition chain mechanism. International Journal of Chemical Kinetics, 1993, 25, 285-303.	1.0	50
54	Separability of Tight and Roaming Pathways to Molecular Decomposition. Journal of Physical Chemistry A, 2012, 116, 6967-6982.	1.1	48

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55	An improved long range potential for O(1D)+H2. Journal of Chemical Physics, 1988, 88, 7653-7661.	1.2	46
56	An ab initio determination of the rate constant for H2+C2Hâ†'H+C2H2. Journal of Chemical Physics, 1982, 76, 5172-5173.	1.2	44
57	Ab initio theoretical results on the stability of cyclic ozone. Journal of Chemical Physics, 1977, 67, 2377.	1.2	43
58	The photoelectron spectroscopy of HOâ^'2. Journal of Chemical Physics, 1985, 83, 5400-5406.	1.2	41
59	Methyl radical:ab initioglobal potential surface, vibrational levels and partition function. Molecular Physics, 2006, 104, 73-81.	0.8	41
60	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
61	Polyatomic surface fitting, vibrational-rotational analysis, expectation value and intensity program. Computer Physics Communications, 1988, 51, 257-284.	3.0	39
62	Unconventional Peroxy Chemistry in Alcohol Oxidation: The Water Elimination Pathway. Journal of Physical Chemistry Letters, 2013, 4, 350-354.	2.1	38
63	Rate Constant and Branching Fraction for the NH₂ + NO₂ Reaction. Journal of Physical Chemistry A, 2013, 117, 9011-9022.	1.1	37
64	Generalized valence bond description of the valence states of formamide. Journal of the American Chemical Society, 1975, 97, 6300-6305.	6.6	36
65	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
66	Theoretical Determination of the Rate Coefficient for the HO_{2Â}+ HO₂ â†' H₂O₂+O₂ Reaction: Adiabatic Treatment of Anharmonic Torsional Effects. Journal of Physical Chemistry A, 2012, 116, 2089-2100.	1.1	35
67	The determination of molecular properties from MULTIMODE with an application to the calculation of Franckâ€"Condon factors for photoionization of CF3to. Molecular Physics, 2006, 104, 33-45.	0.8	34
68	Resolving Some Paradoxes in the Thermal Decomposition Mechanism of Acetaldehyde. Journal of Physical Chemistry A, 2015, 119, 7724-7733.	1.1	33
69	A quasi-classical trajectory study of collisions of fast H atoms with CO using an accurate ab initio potential surface. Chemical Physics Letters, 1985, 114, 520-525.	1.2	32
70	Performance of the Spin-Flip and Multireference Methods for Bond Breaking in Hydrocarbons:â€‰ A Benchmark Study. Journal of Physical Chemistry A, 2007, 111, 13264-13271.	1.1	31
71	Quantum States of the Endohedral Fullerene Li@C₆₀. Journal of Physical Chemistry A, 2008, 112, 5478-5485.	1.1	31
72	Theoretical studies of collisional relaxation of highly excited SO2 in an Ar bath. Faraday Discussions, 1995, 102, 389.	1.6	29

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73	A theoretical study of the kinetics of C2H3+H. Physical Chemistry Chemical Physics, 1999, 1, 989-997.	1.3	28
74	Quasiclassical Trajectory Study of Energy and Angular Distributions for the H + CO2â† ' OH + CO Reactionâ€. Journal of Physical Chemistry B, 2002, 106, 8148-8160.	1.2	28
75	Substitution Reactions in the Pyrolysis of Acetone Revealed through a Modeling, Experiment, Theory Paradigm. Journal of the American Chemical Society, 2021, 143, 3124-3142.	6.6	28
76	A direct transition state theory based analysis of the branching in NH2 + NO. Faraday Discussions, 2001, 119, 207-222.	1.6	27
77	Mechanistic implications of the stereochemistry of singlet oxygen-olefin reactions. Tetrahedron Letters, 1978, 19, 747-750.	0.7	26
78	Interpolating moving least-squares methods for fitting potential energy surfaces: An application to the H2CN unimolecular reaction. Journal of Chemical Physics, 2007, 126, 104105.	1.2	26
79	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
80	The generalized valence bond description of the low-lying states of ketene. Journal of the American Chemical Society, 1976, 98, 6093-6099.	6.6	24
81	Accurate Anharmonic Zero-Point Energies for Some Combustion-Related Species from Diffusion Monte Carlo. Journal of Physical Chemistry A, 2017, 121, 4334-4340.	1.1	22
82	Predictive Theory for the Addition and Insertion Kinetics of ¹CH₂ Reacting with Unsaturated Hydrocarbons. Journal of Physical Chemistry A, 2013, 117, 12677-12692.	1.1	21
83	Comparison of multireference configuration interaction potential energy surfaces for HÂ+ÂO2Ââ†'ÂHO2: the effect of internal contraction. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	21
84	Proton transfers in hydrogen bonded systems. Electron correlation effects in (H3NHOH2)+. Chemical Physics Letters, 1981, 79, 39-42.	1.2	20
85	Importance of hindered rotations in the thermal dissociation of small unsaturated molecules: Classical formulation and application to HCN and HCCH. Journal of Chemical Physics, 1996, 105, 8075-8096.	1.2	20
86	Theoretical study of the reaction rates of OH+OH â‡" H2O+O. Proceedings of the Combustion Institute, 1989, 22, 983-989.	0.3	19
87	A theoretical study of solid hydrogens doped with atomic oxygen. Journal of Chemical Physics, 1997, 106, 942-953.	1.2	19
88	Barrier to Methyl Internal Rotation of 1-Methylvinoxy Radical in the XÌƒ(2Aâ€˜Ââ€˜) and BÌƒ(2Aâ€˜Ââ€˜) States:Â Experiment and Theoryâ€. Journal of Physical Chemistry A, 2000, 104, 10131-10138.	1.1	19
89	Construction of reproducing kernel Hilbert space potential energy surfaces for the 1â€ŠAâ€³ and 1â€ŠAâ€² states of the reaction N(2D)+H2. Journal of Chemical Physics, 2001, 114, 3945-3948.	1.2	19
90	Electronic States of the Quasilinear Molecule Propargylene (HCCCH) from Negative Ion Photoelectron Spectroscopy. Journal of the American Chemical Society, 2014, 136, 10361-10372.	6.6	18

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91	Time-Resolved Kinetic Chirped-Pulse Rotational Spectroscopy in a Room-Temperature Flow Reactor. Journal of Physical Chemistry Letters, 2017, 8, 6180-6188.	2.1	18
92	Inclusion and assessment of Rennerâ€“Teller coupling in transition state theory for Î states: Application to O(3P)+H2. Journal of Chemical Physics, 1985, 82, 1866-1872.	1.2	17
93	Thermal Rate Constant and Branching Ratio for CN + HD â†' HCN/DCN + D/H fromT= 293 to 375 K. Journal of Physical Chemistry A, 1998, 102, 7653-7661.	1.1	17
94	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
95	An ab initio determination of the rate constant for H+H2CO â†'H2+HCO. Journal of Chemical Physics, 1982, 76, 4296-4297.	1.2	15
96	Speciation of C6H6Isomers by Gas Chromatography-Matrix Isolation Fourier Transform Infrared Spectroscopyâ^'Mass Spectrometry. Journal of Physical Chemistry A, 2004, 108, 3403-3405.	1.1	15
97	Direct Measurement and Theoretical Calculation of the Rate Coefficient for Cl + CH3in the Range fromT= 202â^'298 K. Journal of Physical Chemistry A, 2007, 111, 1015-1023.	1.1	15
98	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
99	Barrier to Methyl Internal Rotation of Cis- andTrans-2-Methylvinoxy Radicals in the XÌƒ(2Aâ€˜Ââ€˜) and BÌƒ(2Aâ€˜Ââ€˜) States:Â Experiment and Theory. Journal of Physical Chemistry A, 2000, 104, 9906-9913.	1.1	14
100	Active Thermochemical Tables: The Partition Function of Hydroxymethyl (CH2OH) Revisited. Journal of Physical Chemistry A, 2019, 123, 4212-4231.	1.1	13
101	A Theoretical Study of Reactions on the ClHCN Surface. The Journal of Physical Chemistry, 1996, 100, 10123-10130.	2.9	12
102	Isotope Effects in Addition Reactions of Importance in Combustion. ACS Symposium Series, 1992, , 48-63.	0.5	11
103	The influence of hindered rotations on recombination/dissociation kinetics. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1997, 101, 391-399.	0.9	11
104	REMPI mass spectrum of the OH radical in the gas phase. Chemical Physics Letters, 1991, 183, 465-470.	1.2	10
105	An empirical potential energy surface for the Neâ€“OH/D complexes. Journal of Chemical Physics, 1999, 111, 10053-10060.	1.2	9
106	A Summary of â€œA Direct Transition State Theory Based Study of Methyl Radical Recombination Kineticsâ€• Journal of Physical Chemistry A, 2000, 104, 2351-2354.	1.1	9
107	Reaction Profiles and Kinetics for Radicalâ€“Radical Hydrogen Abstraction via Multireference Coupled Cluster Theory. Journal of Chemical Theory and Computation, 2020, 16, 1511-1525.	2.3	8
108	Secondary channels in the thermal decomposition of monomethylhydrazine (CH3NHNH2). RSC Advances, 2014, 4, 62951-62964.	1.7	3

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109	Comment on â€œA novel and facile decay path of Criegee intermediates by intramolecular insertion reactions via roaming transition statesâ€•[J. Chem. Phys. 142, 124312 (2015)]. Journal of Chemical Physics, 2015, 143, 167101.	1.2	3
110	Quantum chemical calculations using the floating point systems, Inc. Model 164 attached processor. International Journal of Quantum Chemistry, 1983, 24, 613-622.	1.0	2
111	Approximate Quantum Approaches to the Calculation of Resonances in Reactive and Nonreactive Scattering. ACS Symposium Series, 1984, , 43-62.	0.5	1
112	Autobiography of Lawrence B. Harding. Journal of Physical Chemistry A, 2015, 119, 7078-7079.	1.1	0