Joel Bowman

List of Publications by Year
in descending order

352 papers	20,056 citations	10373 72 h-index	17090 122 g-index
358 all docs	358 docs citations	358 times ranked	5717 citing authors

#	Article	IF	Citations
1	Permutationally invariant potential energy surfaces in high dimensionality. International Reviews in Physical Chemistry, 2009, 28, 577-606.	0.9	730
2	Selfâ€consistent field energies and wavefunctions for coupled oscillators. Journal of Chemical Physics, 1978, 68, 608-610.	1.2	554
3	The self-consistent-field approach to polyatomic vibrations. Accounts of Chemical Research, 1986, 19, 202-208.	7.6	541
4	The Roaming Atom: Straying from the Reaction Path in Formaldehyde Decomposition. Science, 2004, 306, 1158-1161.	6.0	538
5	Vibrational self-consistent field method for many-mode systems: A new approach and application to the vibrations of CO adsorbed on Cu(100). Journal of Chemical Physics, 1997, 107, 10458-10469.	1.2	501
6	Reduced dimensionality theory of quantum reactive scattering. The Journal of Physical Chemistry, 1991, 95, 4960-4968.	2.9	435
7	MULTIMODE: A code to calculate rovibrational energies of polyatomic molecules. International Reviews in Physical Chemistry, 2003, 22, 533-549.	0.9	413
8	Variational quantum approaches for computing vibrational energies of polyatomic molecules. Molecular Physics, 2008, 106, 2145-2182.	0.8	402
9	Extensions and tests of "multimode": a code to obtain accurate vibration/rotation energies of many-mode molecules. Theoretical Chemistry Accounts, 1998, 100, 191-198.	0.5	393
10	Investigations of self-consistent field, scf ci and virtual stateconfiguration interaction vibrational energies for a model three-mode system. Chemical Physics Letters, 1982, 85, 220-224.	1.2	275
11	Ab initio potential energy and dipole moment surfaces for H5O2+. Journal of Chemical Physics, 2005, 122, 044308.	1.2	257
12	High-dimensional ab initio potential energy surfaces for reaction dynamics calculations. Physical Chemistry Chemical Physics, 2011, 13, 8094.	1.3	252
13	Permutationally Invariant Polynomial Basis for Molecular Energy Surface Fitting via Monomial Symmetrization. Journal of Chemical Theory and Computation, 2010, 6, 26-34.	2.3	249
14	Flexible, ab initio potential, and dipole moment surfaces for water. I. Tests and applications for clusters up to the 22-mer. Journal of Chemical Physics, 2011, 134, 094509.	1.2	238
15	The vibrational predissociation spectra of the H5O2+â‹™RGn(RG=Ar,Ne) clusters: Correlation of the solvent perturbations in the free OH and shared proton transitions of the Zundel ion. Journal of Chemical Physics, 2005, 122, 244301.	1.2	228
16	Ab initio calculations of electronic and vibrational energies of HCO and HOC. Journal of Chemical Physics, 1986, 85, 911-921.	1.2	216
17	Roaming Radicals. Annual Review of Physical Chemistry, 2011, 62, 531-553.	4.8	189
18	Vibrational energy levels of formaldehyde. Journal of Chemical Physics, 1985, 82, 4155-4165.	1.2	187

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19	Roaming is the dominant mechanism for molecular products in acetaldehyde photodissociation. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 12719-12724.	3.3	183
20	Ab initiocalculation of a global potential, vibrational energies, and wave functions for HCN/HNC, and a simulation of theAÌƒâ€“XÌƒ emission spectrum. Journal of Chemical Physics, 1993, 99, 308-323.	1.2	174
21	Dynamics of the Reaction of Methane with Chlorine Atom on an Accurate Potential Energy Surface. Science, 2011, 334, 343-346.	6.0	167
22	Accurate ab initio and â€œhybridâ€•potential energy surfaces, intramolecular vibrational energies, and classical ir spectrum of the water dimer. Journal of Chemical Physics, 2009, 130, 144314.	1.2	162
23	A method to constrain vibrational energy in quasiclassical trajectory calculations. Journal of Chemical Physics, 1989, 91, 2859-2862.	1.2	152
24	Permutationally Invariant Potential Energy Surfaces. Annual Review of Physical Chemistry, 2018, 69, 151-175.	4.8	152
25	Full-dimensional quantum calculations of ground-state tunneling splitting of malonaldehyde using an accurate ab initio potential energy surface. Journal of Chemical Physics, 2008, 128, 224314.	1.2	149
26	Unimolecular dissociation dynamics of vibrationally activated CH3CHOO Criegee intermediates to OH radical products. Nature Chemistry, 2016, 8, 509-514.	6.6	141
27	Ab initio potential and dipole moment surfaces for water. II. Local-monomer calculations of the infrared spectra of water clusters. Journal of Chemical Physics, 2011, 134, 154510.	1.2	136
28	A Global ab Initio Potential Energy Surface for Formaldehydeâ€. Journal of Physical Chemistry A, 2004, 108, 8980-8986.	1.1	135
29	Full-dimensional, ab initio potential energy and dipole moment surfaces for water. Journal of Chemical Physics, 2009, 131, 054511.	1.2	133
30	The Water Hexamer: Cage, Prism, or Both. Full Dimensional Quantum Simulations Say Both. Journal of the American Chemical Society, 2012, 134, 11116-11119.	6.6	132
31	Crossover from hydrogen to chemical bonding. Science, 2021, 371, 160-164.	6.0	123
32	Ab Initio Potential Energy and Dipole Moment Surfaces of (H2O)2â€. Journal of Physical Chemistry A, 2006, 110, 445-451.	1.1	115
33	Roaming. Molecular Physics, 2014, 112, 2516-2528.	0.8	113
34	Reduced dimensionality quantum reactive scattering: H2+CNâ†'H+HCN. Journal of Chemical Physics, 1990, 92, 5201-5210.	1.2	111
35	The adiabatic rotation approximation for rovibrational energies of many-mode systems: Description and tests of the method. Journal of Chemical Physics, 1998, 108, 4397-4404.	1.2	111
36	An accurateab initioHOCl potential energy surface, vibrational and rotational calculations, and comparison with experiment. Journal of Chemical Physics, 1998, 109, 2662-2671.	1.2	110

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37	Ab initio global potential-energy surface for H5+â†'H3++H2. Journal of Chemical Physics, 2005, 122, 224307.	1.2	106
38	A reduced dimensionality, six-degree-of-freedom, quantum calculation of the H+CH4â†'H2+CH3 reaction. Journal of Chemical Physics, 2001, 115, 2055-2061.	1.2	104
39	New ab initio potential energy surface and the vibration-rotation-tunneling levels of (H2O)2 and (D2O)2. Journal of Chemical Physics, 2008, 128, 034312.	1.2	104
40	A truncation/recoupling method for basis set calculations of eigenvalues and eigenvectors. Journal of Chemical Physics, 1991, 94, 454-460.	1.2	103
41	Intersystem crossing and dynamics in O(³ P)Â+ÂC ₂ H ₄ multichannel reaction: Experiment validates theory. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 9733-9738.	3.3	102
42	Communication: A chemically accurate global potential energy surface for the HO + CO â†' H + CO2 reaction. Journal of Chemical Physics, 2012, 136, 041103.	1.2	102
43	Sudden rotation reactive scattering: Theory and application to 3â€Ð H+H2. Journal of Chemical Physics, 1980, 72, 5071-5088.	1.2	98
44	Classical and quasiclassical spectral analysis of CH5+ using an ab initio potential energy surface. Journal of Chemical Physics, 2003, 119, 8790-8793.	1.2	97
45	Full-dimensional vibrational calculations for H5O2+ using an ab initio potential energy surface. Journal of Chemical Physics, 2005, 122, 061101.	1.2	97
46	An ab Initio Based Global Potential Energy Surface Describing CH5+â†' CH3++ H2â€. Journal of Physical Chemistry A, 2006, 110, 1569-1574.	1.1	97
47	Ab-Initio-Based Potential Energy Surfaces for Complex Molecules and Molecular Complexes. Journal of Physical Chemistry Letters, 2010, 1, 1866-1874.	2.1	97
48	Reaction Dynamics of Methane with F, O, Cl, and Br on ab Initio Potential Energy Surfaces. Journal of Physical Chemistry A, 2014, 118, 2839-2864.	1.1	96
49	Reduced Dimensionality Theories of Quantum Reactive Scattering. Advances in Chemical Physics, 2007, , 115-167.	0.3	93
50	Vibrational Analysis of the H5O2+ Infrared Spectrum Using Molecular and Driven Molecular Dynamics. Journal of Physical Chemistry A, 2006, 110, 2933-2939.	1.1	91
51	Mode selectivity in reactions of H with HOD(100), HOD(001), and HOD(002). Journal of Chemical Physics, 1992, 96, 7852-7854.	1.2	90
52	Three-State Trajectory Surface Hopping Studies of the Photodissociation Dynamics of Formaldehyde on ab Initio Potential Energy Surfaces. Journal of the American Chemical Society, 2011, 133, 7957-7968.	6.6	90
53	Experimental and reduced dimensionality quantum rate coefficients for H2(D2)+CNâ†'H(D)CN+H(D). Journal of Chemical Physics, 1990, 93, 4730-4739.	1.2	89
54	Variational calculations of rovibrational energies of CH4 and isotopomers in full dimensionality using an ab initio potential. Journal of Chemical Physics, 1999, 110, 8417-8423.	1.2	89

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55	A wave-packet calculation of the effect of reactant rotation and alignment on product branching in the O(1D)+HClâ†'ClO+H, OH+Cl reactions. Journal of Chemical Physics, 2000, 113, 1-3.	1.2	89
56	Quasiclassical Trajectory Calculations of Acetaldehyde Dissociation on a Global Potential Energy Surface Indicate Significant Non-transition State Dynamics. Journal of Physical Chemistry A, 2007, 111, 8282-8285.	1.1	89
57	Experimental and Theoretical Investigations of Energy Transfer and Hydrogen-Bond Breaking in the Water Dimer. Journal of the American Chemical Society, 2012, 134, 15430-15435.	6.6	89
58	Î" -machine learning for potential energy surfaces: A PIP approach to bring a DFT-based PES to CCSD(T) level of theory. Journal of Chemical Physics, 2021, 154, 051102.	1.2	89
59	Ab Initio Diffusion Monte Carlo Calculations of the Quantum Behavior of CH5+ in Full Dimensionality. Journal of Physical Chemistry A, 2004, 108, 4991-4994.	1.1	87
60	Mode Selectivity for a â€œCentralâ€•Barrier Reaction: Eight-Dimensional Quantum Studies of the O(³P) + CH₄ â†' OH + CH₃ Reaction on an Ab Initio Potential Energy Surface. Journal of Physical Chemistry Letters, 2012, 3, 3776-3780.	2.1	87
61	High-Level, First-Principles, Full-Dimensional Quantum Calculation of the Ro-vibrational Spectrum of the Simplest Criegee Intermediate (CH₂OO). Journal of Physical Chemistry Letters, 2014, 5, 2364-2369.	2.1	86
62	â€œRoamingâ€•Dynamics in CH₃CHO Photodissociation Revealed on a Global Potential Energy Surface. Journal of Physical Chemistry A, 2008, 112, 9344-9351.	1.1	84
63	A theoretical study of the vibrational energy spectrum of the HOCl/HClO system on an accurate ab initio potential energy surface. Journal of Chemical Physics, 1999, 111, 7446-7456.	1.2	83
64	The roaming atom pathway in formaldehyde decomposition. Journal of Chemical Physics, 2006, 125, 044303.	1.2	83
65	Structure, Anharmonic Vibrational Frequencies, and Intensities of NNHNN⁺. Journal of Physical Chemistry A, 2015, 119, 11623-11631.	1.1	81
66	Complex coordinate calculations of Feshbach resonance energies and widths for a collinear triatomic system. Journal of Chemical Physics, 1983, 78, 3952-3958.	1.2	80
67	A theoretical study of vibrational mode coupling in H5O2+. Journal of Chemical Physics, 2003, 119, 6571-6580.	1.2	79
68	Assessing Gaussian Process Regression and Permutationally Invariant Polynomial Approaches To Represent High-Dimensional Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2018, 14, 3381-3396.	2.3	78
69	Reduced dimensionality quantum calculations of mode specificity in OH+H2â†"H2O+H. Journal of Chemical Physics, 1992, 96, 8906-8913.	1.2	77
70	An ab initio potential energy surface for the formic acid dimer: zero-point energy, selected anharmonic fundamental energies, and ground-state tunneling splitting calculated in relaxed 1â€“4-mode subspaces. Physical Chemistry Chemical Physics, 2016, 18, 24835-24840.	1.3	76
71	Sudden rotation calculations of atomâ€“molecule scattering. Journal of Chemical Physics, 1977, 66, 288-295.	1.2	75
72	Roaming reactions: The third way. Physics Today, 2011, 64, 33-37.	0.3	75

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73	L2 calculations of resonances and final rotational distributions for HCOâ†'H+CO. Journal of Chemical Physics, 1994, 100, 1021-1027.	1.2	74
74	Communication: On the consistency of approximate quantum dynamics simulation methods for vibrational spectra in the condensed phase. Journal of Chemical Physics, 2014, 141, 181101.	1.2	74
75	Infrared identification of the Criegee intermediates syn- and anti-CH3CHOO, and their distinct conformation-dependent reactivity. Nature Communications, 2015, 6, 7012.	5.8	74
76	A simple method to adjust potential energy surfaces: Application to HCO. Journal of Chemical Physics, 1991, 94, 816-817.	1.2	71
77	New insights on reaction dynamics from formaldehyde photodissociation. Physical Chemistry Chemical Physics, 2006, 8, 321-332.	1.3	69
78	Differences in the Vibrational Dynamics of H₂O and D₂O: Observation of Symmetric and Antisymmetric Stretching Vibrations in Heavy Water. Journal of Physical Chemistry Letters, 2016, 7, 1769-1774.	2.1	68
79	Coupled channel calculation of resonances in H+CO. Journal of Chemical Physics, 1986, 84, 4888-4893.	1.2	67
80	Full-dimensionality quantum calculations of acetyleneâ€"vinylidene isomerization. Journal of Chemical Physics, 2003, 118, 10012-10023.	1.2	67
81	Signatures of H2CO Photodissociation from Two Electronic States. Science, 2006, 311, 1443-1446.	6.0	67
82	Theories and simulations of roaming. Chemical Society Reviews, 2017, 46, 7615-7624.	18.7	67
83	Resonances:Â Bridge between Spectroscopy and Dynamics. Journal of Physical Chemistry A, 1998, 102, 3006-3017.	1.1	65
84	Directab initiovariational calculation of vibrational energies of the H2Oâ‹¯Clâ¯' complex and resolution of experimental differences. Journal of Chemical Physics, 2000, 113, 8401-8403.	1.2	64
85	Quasiclassical trajectory study of formaldehyde unimolecular dissociation: H2COâ†'H2+CO, H+HCO. Journal of Chemical Physics, 2005, 122, 114313.	1.2	63
86	An adjusted global potential surface for HCN based on rigorous vibrational calculations. Journal of Chemical Physics, 1991, 95, 6309-6316.	1.2	62
87	Calculations of rovibrational energies and dipole transition intensities for polyatomic molecules using <scp>MULTIMODE</scp>. Journal of Chemical Physics, 2009, 131, 224106.	1.2	62
88	Roaming Pathway Leading to Unexpected Water + Vinyl Products in C₂H₄OH Dissociation. Journal of Physical Chemistry Letters, 2010, 1, 3058-3065.	2.1	62
89	Quantum calculations of mode specificity in reactions of H with HOD and H2O. Journal of Chemical Physics, 1993, 98, 6235-6247.	1.2	61
90	Ab initio potential energy surface and rovibrational energies of H3O+ and its isotopomers. Journal of Chemical Physics, 2003, 118, 5431-5441.	1.2	61

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91	Vibrational Levels of Methanol Calculated by the Reaction Path Version of MULTIMODE, Using an ab initio, Full-Dimensional Potentialâ€. Journal of Physical Chemistry A, 2007, 111, 7317-7321.	1.1	61
92	Quantum dynamics of COâ€“H2 in full dimensionality. Nature Communications, 2015, 6, 6629.	5.8	61
93	Capturing roaming molecular fragments in real time. Science, 2020, 370, 1072-1077.	6.0	61
94	Permutationally Invariant Fitting of Many-Body, Non-covalent Interactions with Application to Three-Body Methaneâ€“Waterâ€“Water. Journal of Chemical Theory and Computation, 2015, 11, 1631-1638.	2.3	60
95	Resonances in the O(3P)+HCl reaction due to van der Waals minima. Journal of Chemical Physics, 2002, 116, 7461-7467.	1.2	59
96	Overview of reduced dimensionality quantum approaches to reactive scattering. Theoretical Chemistry Accounts, 2002, 108, 125-133.	0.5	59
97	A comparative study of the reaction dynamics of several potential energy surfaces of O(3P)+H2â†'OH+H. I. Journal of Chemical Physics, 1981, 74, 4984-4996.	1.2	58
98	Argon Predissociation Spectroscopy of the OH-Â·H2O and Cl-Â·H2O Complexes in the 1000â^'1900 cm-1Region:Â Intramolecular Bending Transitions and the Search for the Shared-Proton Fundamental in the Hydroxide Monohydrate. Journal of Physical Chemistry A, 2005, 109, 571-575.	1.1	56
99	Communication: VSCF/VCI vibrational spectroscopy of H7O3+ and H9O4+ using high-level, many-body potential energy surface and dipole moment surfaces. Journal of Chemical Physics, 2017, 146, 121102.	1.2	56
100	A threeâ€dimensional L2 simulation of the photodetachment spectra of ClHClâ^' and IHIâ^'. Journal of Chemical Physics, 1989, 91, 4615-4624.	1.2	55
101	Vibrational spectrum of the formic acid dimer in the OH stretch region. A model 3D study. Chemical Physics Letters, 2001, 349, 562-570.	1.2	55
102	IR Spectra of the Water Hexamer: Theory, with Inclusion of the Monomer Bend Overtone, and Experiment Are in Agreement. Journal of Physical Chemistry Letters, 2013, 4, 1104-1108.	2.1	55
103	Quasiclassical Trajectory Study of CH₃NO₂ Decomposition via Roaming Mediated Isomerization Using a Global Potential Energy Surface. Journal of Physical Chemistry A, 2013, 117, 11665-11672.	1.1	54
104	â€œPlug and playâ€•full-dimensional ab initio potential energy and dipole moment surfaces and anharmonic vibrational analysis for CH₄â€“H₂O. Physical Chemistry Chemical Physics, 2015, 17, 8172-8181.	1.3	54
105	Energy dependence of the roaming atom pathway in formaldehyde decomposition. Journal of Chemical Physics, 2007, 126, 044314.	1.2	53
106	The internal coordinate path Hamiltonian; application to methanol and malonaldehyde. Molecular Physics, 2003, 101, 3513-3525.	0.8	51
107	Reaction dynamics for O(3P)+H2 and D2. IV. Reduced dimensionality quantum and quasiclassical rate constants with an adiabatic incorporation of the bending motion. Journal of Chemical Physics, 1984, 81, 1739-1752.	1.2	49
108	Quasiclassical trajectory study of the postquenching dynamics of OHâ€‰Å£2+ by H2/D2 on a global potential energy surface. Journal of Chemical Physics, 2010, 133, 164306.	1.2	49

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109	Crossed Molecular Beams and Quasiclassical Trajectory Surface Hopping Studies of the Multichannel Nonadiabatic O(³P) + Ethylene Reaction at High Collision Energy. Journal of Physical Chemistry A, 2015, 119, 12498-12511.	1.1	49
110	Energetics and Predissociation Dynamics of Small Water, HCl, and Mixed HClâ€“Water Clusters. Chemical Reviews, 2016, 116, 4913-4936.	23.0	49
111	The infrared spectrum of the hydrogen bifluoride anion: unprecedented variation with level of theory. Chemical Physics Letters, 1986, 131, 352-358.	1.2	48
112	A comparative study of the reaction dynamics of several potential energy surfaces for O(3P)+H2â€‰â†’â€‰OH+H. II. Collinear exact quantum and quasiclassical reaction probabilities. Journal of Chemical Physics, 1982, 76, 3563-3582.	1.2	47
113	The effect of rotation on resonances: Application to HCO. Journal of Chemical Physics, 1996, 105, 9884-9889.	1.2	47
114	Photodissociation dynamics of nitromethane and methyl nitrite by infrared multiphoton dissociation imaging with quasiclassical trajectory calculations: Signatures of the roaming pathway. Journal of Chemical Physics, 2014, 140, 054305.	1.2	47
115	Three Reaction Pathways in the H + HCO â†’ H₂ + CO Reaction. Journal of Physical Chemistry A, 2009, 113, 4138-4144.	1.1	46
116	Coupled-monomers in molecular assemblies: Theory and application to the water tetramer, pentamer, and ring hexamer. Journal of Chemical Physics, 2012, 136, 144113.	1.2	46
117	Experimental and Theoretical Investigations of the Dissociation Energy (D0) and Dynamics of the Water Trimer, (H2O)3. Journal of Physical Chemistry A, 2013, 117, 7207-7216.	1.1	46
118	Experimental and Theoretical Investigations of Energy Transfer and Hydrogen-Bond Breaking in Small Water and HCl Clusters. Accounts of Chemical Research, 2014, 47, 2700-2709.	7.6	46
119	Quantum calculations of the IR spectrum of liquid water using ab initio and model potential and dipole moment surfaces and comparison with experiment. Journal of Chemical Physics, 2015, 142, 194502.	1.2	46
120	Vibrational analysis of HOCl up to 98% of the dissociation energy with a Fermi resonance Hamiltonian. Journal of Chemical Physics, 1999, 111, 6807-6820.	1.2	45
121	Roaming Under the Microscope: Trajectory Study of Formaldehyde Dissociation. Journal of Physical Chemistry A, 2016, 120, 5103-5114.	1.1	45
122	The calculated infrared spectrum of Clâ¯H2O using a new full dimensionalab initiopotential surface and dipole moment surface. Journal of Chemical Physics, 2006, 125, 133206.	1.2	44
123	Are Roaming and Conventional Saddle Points for H₂CO and CH₃CHO Dissociation to Molecular Products Isolated from Each Other?. Journal of Physical Chemistry Letters, 2011, 2, 834-838.	2.1	44
124	Mode-specific tunneling using the Qim path: Theory and an application to full-dimensional malonaldehyde. Journal of Chemical Physics, 2013, 139, 154303.	1.2	44
125	Disentangling the Complex Vibrational Spectrum of the Protonated Water Trimer, H⁺(H₂O)₃, with Two-Color IR-IR Photodissociation of the Bare Ion and Anharmonic VSCF/VCI Theory. Journal of Physical Chemistry Letters, 2017, 8, 3782-3789.	2.1	44
126	Quantum and classical dynamics of a coupled double well oscillator. Journal of Chemical Physics, 1981, 74, 5057-5075.	1.2	43

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127	High-Level Quantum Calculations of the IR Spectra of the Eigen, Zundel, and Ring Isomers of H⁺(H₂O)₄ Find a Single Match to Experiment. Journal of the American Chemical Society, 2017, 139, 10984-10987.	6.6	43
128	Using Gradients in Permutationally Invariant Polynomial Potential Fitting: A Demonstration for CH₄ Using as Few as 100 Configurations. Journal of Chemical Theory and Computation, 2019, 15, 2826-2835.	2.3	43
129	Quasiclassical trajectory studies of rigid rotorâ€“rigid surface scattering. I. Flat surface. Journal of Chemical Physics, 1982, 77, 5441-5449.	1.2	42
130	Quantum calculations of the rate constant for the O(3P)+HCl reaction on new ab initio 3Aâ€³ and 3Aâ€² surfaces. Journal of Chemical Physics, 2003, 119, 9601-9608.	1.2	42
131	Communication: Spectroscopic consequences of proton delocalization in OCHCO+. Journal of Chemical Physics, 2015, 143, 071102.	1.2	42
132	A Machine Learning Approach for Prediction of Rate Constants. Journal of Physical Chemistry Letters, 2019, 10, 5250-5258.	2.1	42
133	New approximate quantum cross sections for the H+H2 reaction. Journal of Chemical Physics, 1981, 75, 5199-5201.	1.2	41
134	A comparative study of the reaction dynamics of the O(3P)+H2â€‰â†’â€‰OH+H reaction on several potential energy surfaces. III. Collinear exact quantum transmission coefficient correction to transition state theory. Journal of Chemical Physics, 1982, 76, 3583-3596.	1.2	41
135	Theoretical studies of the reactivity and spectroscopy of H+CO=HCO. I. Stabilization and scattering studies of resonances for J=0 on the Harding ab initio surface. Journal of Chemical Physics, 1992, 96, 2799-2811.	1.2	41
136	Mid- and Far-IR Spectra of H₅⁺ and D₅⁺ Compared to the Predictions of Anharmonic Theory. Journal of Physical Chemistry Letters, 2012, 3, 3160-3166.	2.1	41
137	q-AQUA: A Many-Body CCSD(T) Water Potential, Including Four-Body Interactions, Demonstrates the Quantum Nature of Water from Clusters to the Liquid Phase. Journal of Physical Chemistry Letters, 2022, 13, 5068-5074.	2.1	41
138	One-dimensional tunneling calculations in the imaginary-frequency, rectilinear saddle-point normal mode. Journal of Chemical Physics, 2008, 129, 121103.	1.2	40
139	Evidence for Vinylidene Production in the Photodissociation of the Allyl Radical. Journal of Physical Chemistry Letters, 2010, 1, 1875-1880.	2.1	40
140	Quasiclassical Trajectory Calculations of the Dissociation Dynamics of CH₃CHO at High Energy Yield Many Products. Journal of Physical Chemistry Letters, 2011, 2, 1715-1719.	2.1	40
141	Full-dimensional, high-level ab initio potential energy surfaces for H2(H2O) and H2(H2O)2 with application to hydrogen clathrate hydrates. Journal of Chemical Physics, 2015, 143, 084302.	1.2	40
142	Normal-mode analysis without the Hessian: A driven molecular-dynamics approach. Journal of Chemical Physics, 2003, 119, 646-650.	1.2	39
143	First-principles calculations of rovibrational energies, dipole transition intensities and partition function for ethylene using MULTIMODE. Journal of Chemical Physics, 2012, 137, 154301.	1.2	39
144	Benchmark Electronic Structure Calculations for H₃O⁺(H₂O)_n, n = 0â€“5, Clusters and Tests of an Existing 1,2,3-Body Potential Energy Surface with a New 4-Body Correction. Journal of Chemical Theory and Computation, 2018, 14, 4553-4566.	2.3	39

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145	Breaking the Coupled Cluster Barrier for Machine-Learned Potentials of Large Molecules: The Case of 15-Atom Acetylacetone. Journal of Physical Chemistry Letters, 2021, 12, 4902-4909.	2.1	39
146	A movable basis method to calculate vibrational energies of molecules. Journal of Chemical Physics, 1990, 93, 1774-1784.	1.2	38
147	Quantum calculations of unusual mode specificity in H+C2H2â†'H2+C2H. Journal of Chemical Physics, 1994, 101, 8646-8662.	1.2	38
148	Skirting the transition state, a new paradigm in reaction rate theory. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 16061-16062.	3.3	38
149	Deconstructing Prominent Bands in the Terahertz Spectra of H7O3+ and H9O4+: Intermolecular Modes in Eigen Clusters. Journal of Physical Chemistry Letters, 2018, 9, 798-803.	2.1	38
150	Recovering a full dimensional quantum rate constant from a reduced dimensionality calculation: Application to the OH+COâ†'H+CO2 reaction. Journal of Chemical Physics, 1996, 105, 2280-2286.	1.2	37
151	Full dimensionality quantum calculations of acetylene/vinylidene isomerization. Journal of Chemical Physics, 2002, 117, 5507-5510.	1.2	37
152	Ab Initio Potential Energy Surface and Vibrational Energies of H3O+and Its Isotopomersâ€. Journal of Physical Chemistry B, 2002, 106, 8182-8188.	1.2	37
153	Communication: A benchmark-quality, full-dimensional ab initio potential energy surface for Ar-HOCO. Journal of Chemical Physics, 2014, 140, .	1.2	37
154	A fragmented, permutationally invariant polynomial approach for potential energy surfaces of large molecules: Application to N-methyl acetamide. Journal of Chemical Physics, 2019, 150, 141101.	1.2	37
155	Vibrational dynamics up to the dissociation threshold: A case study of two-dimensional HOCl. Journal of Chemical Physics, 2000, 113, 9610-9621.	1.2	36
156	Quantum Calculations of Intramolecular IR Spectra of Ice Models Using Ab Initio Potential and Dipole Moment Surfaces. Journal of Physical Chemistry Letters, 2012, 3, 3671-3676.	2.1	36
157	Quantum approaches to vibrational dynamics and spectroscopy: is ease of interpretation sacrificed as rigor increases?. Physical Chemistry Chemical Physics, 2019, 21, 3397-3413.	1.3	35
158	Quasiclassical studies of rigid rotorâ€"solid surface diffraction scattering. Journal of Chemical Physics, 1977, 66, 1122-1126.	1.2	34
159	Perturbative inversion of the HOCl potential energy surface via singular value decomposition. Chemical Physics Letters, 1999, 312, 494-502.	1.2	34
160	CHEMISTRY: Beyond Platonic Molecules. Science, 2000, 290, 724-725.	6.0	34
161	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
162	Photodissociation Dynamics of Formaldehyde Initiated at the T₁/S₀ Minimum Energy Crossing Configurations. Journal of Physical Chemistry A, 2008, 112, 13267-13270.	1.1	34

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