

Joel Bowman

List of Publications by Year in descending order

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352
papers

20,056
citations

10389

72
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17105

122
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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.	2.3	730
2	Self-consistent field energies and wavefunctions for coupled oscillators. Journal of Chemical Physics, 1978, 68, 608-610.	3.0	554
3	The self-consistent-field approach to polyatomic vibrations. Accounts of Chemical Research, 1986, 19, 202-208.	15.6	541
4	The Roaming Atom: Straying from the Reaction Path in Formaldehyde Decomposition. Science, 2004, 306, 1158-1161.	12.6	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.	3.0	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.	2.3	413
8	Variational quantum approaches for computing vibrational energies of polyatomic molecules. Molecular Physics, 2008, 106, 2145-2182.	1.7	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.	1.4	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.	2.6	275
11	Ab initio potential energy and dipole moment surfaces for H ₅ O ₂ ⁺ . Journal of Chemical Physics, 2005, 122, 044308.	3.0	257
12	High-dimensional ab initio potential energy surfaces for reaction dynamics calculations. Physical Chemistry Chemical Physics, 2011, 13, 8094.	2.8	252
13	Permutationally Invariant Polynomial Basis for Molecular Energy Surface Fitting via Monomial Symmetrization. Journal of Chemical Theory and Computation, 2010, 6, 26-34.	5.3	249
14	Flexible, <i>ab initio</i> 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.	3.0	238
15	The vibrational predissociation spectra of the H ₅ O ₂ ⁺ + TM RG _n (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.	3.0	228
16	Ab initio calculations of electronic and vibrational energies of HCO and HOC. Journal of Chemical Physics, 1986, 85, 911-921.	3.0	216
17	Roaming Radicals. Annual Review of Physical Chemistry, 2011, 62, 531-553.	10.8	189
18	Vibrational energy levels of formaldehyde. Journal of Chemical Physics, 1985, 82, 4155-4165.	3.0	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.	7.1	183
20	Ab initio calculation of a global potential, vibrational energies, and wave functions for HCN/HNC, and a simulation of the $\text{A}^1\Sigma^+$ emission spectrum. Journal of Chemical Physics, 1993, 99, 308-323.	3.0	174
21	Dynamics of the Reaction of Methane with Chlorine Atom on an Accurate Potential Energy Surface. Science, 2011, 334, 343-346.	12.6	167
22	Accurate <i>ab initio</i> and ρ -hybrid potential energy surfaces, intramolecular vibrational energies, and classical ir spectrum of the water dimer. Journal of Chemical Physics, 2009, 130, 144314.	3.0	162
23	A method to constrain vibrational energy in quasiclassical trajectory calculations. Journal of Chemical Physics, 1989, 91, 2859-2862.	3.0	152
24	Permutationally Invariant Potential Energy Surfaces. Annual Review of Physical Chemistry, 2018, 69, 151-175.	10.8	152
25	Full-dimensional quantum calculations of ground-state tunneling splitting of malonaldehyde using an accurate <i>ab initio</i> potential energy surface. Journal of Chemical Physics, 2008, 128, 224314.	3.0	149
26	Unimolecular dissociation dynamics of vibrationally activated CH_3CHOO Criegee intermediates to OH radical products. Nature Chemistry, 2016, 8, 509-514.	13.6	141
27	<i>Ab initio</i> 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.	3.0	136
28	A Global <i>ab Initio</i> Potential Energy Surface for Formaldehyde. Journal of Physical Chemistry A, 2004, 108, 8980-8986.	2.5	135
29	Full-dimensional, <i>ab initio</i> potential energy and dipole moment surfaces for water. Journal of Chemical Physics, 2009, 131, 054511.	3.0	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.	13.7	132
31	Crossover from hydrogen to chemical bonding. Science, 2021, 371, 160-164.	12.6	123
32	<i>Ab Initio</i> Potential Energy and Dipole Moment Surfaces of $(\text{H}_2\text{O})_2$. Journal of Physical Chemistry A, 2006, 110, 445-451.	2.5	115
33	Roaming. Molecular Physics, 2014, 112, 2516-2528.	1.7	113
34	Reduced dimensionality quantum reactive scattering: $\text{H}_2 + \text{CN}^+ \rightarrow \text{H} + \text{HCN}$. Journal of Chemical Physics, 1990, 92, 5201-5210.	3.0	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.	3.0	111
36	An accurate <i>ab initio</i> HOCl potential energy surface, vibrational and rotational calculations, and comparison with experiment. Journal of Chemical Physics, 1998, 109, 2662-2671.	3.0	110

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37	Ab initio global potential-energy surface for $\text{H}_5+\text{H}_3\rightarrow\text{H}_2$. Journal of Chemical Physics, 2005, 122, 224307.	3.0	106
38	A reduced dimensionality, six-degree-of-freedom, quantum calculation of the $\text{H}+\text{CH}_4\rightarrow\text{H}_2+\text{CH}_3$ reaction. Journal of Chemical Physics, 2001, 115, 2055-2061.	3.0	104
39	New <i>ab initio</i> potential energy surface and the vibration-rotation-tunneling levels of $(\text{H}_2\text{O})_2$ and $(\text{D}_2\text{O})_2$. Journal of Chemical Physics, 2008, 128, 034312.	3.0	104
40	A truncation/recoupling method for basis set calculations of eigenvalues and eigenvectors. Journal of Chemical Physics, 1991, 94, 454-460.	3.0	103
41	Intersystem crossing and dynamics in $\text{O}(\text{ }^3\text{P})+\text{H}_2\text{O} \rightarrow \text{H}_2\text{O}_2+\text{H}$ multichannel reaction: Experiment validates theory. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 9733-9738.	7.1	102
42	Communication: A chemically accurate global potential energy surface for the $\text{HO}+\text{CO} \rightarrow \text{H}+\text{CO}_2$ reaction. Journal of Chemical Physics, 2012, 136, 041103.	3.0	102
43	Sudden rotation reactive scattering: Theory and application to $3\text{D}+\text{H}_2$. Journal of Chemical Physics, 1980, 72, 5071-5088.	3.0	98
44	Classical and quasiclassical spectral analysis of CH_5^+ using an <i>ab initio</i> potential energy surface. Journal of Chemical Physics, 2003, 119, 8790-8793.	3.0	97
45	Full-dimensional vibrational calculations for H_5O_2^+ using an <i>ab initio</i> potential energy surface. Journal of Chemical Physics, 2005, 122, 061101.	3.0	97
46	An <i>ab Initio</i> Based Global Potential Energy Surface Describing $\text{CH}_5+\text{CH}_3\rightarrow\text{H}_2+\text{C}_2\text{H}_6$. Journal of Physical Chemistry A, 2006, 110, 1569-1574.	2.5	97
47	Ab-Initio-Based Potential Energy Surfaces for Complex Molecules and Molecular Complexes. Journal of Physical Chemistry Letters, 2010, 1, 1866-1874.	4.6	97
48	Reaction Dynamics of Methane with F, O, Cl, and Br on <i>ab Initio</i> Potential Energy Surfaces. Journal of Physical Chemistry A, 2014, 118, 2839-2864.	2.5	96
49	Reduced Dimensionality Theories of Quantum Reactive Scattering. Advances in Chemical Physics, 2007, , 115-167.	0.3	93
50	Vibrational Analysis of the H_5O_2^+ Infrared Spectrum Using Molecular and Driven Molecular Dynamics. Journal of Physical Chemistry A, 2006, 110, 2933-2939.	2.5	91
51	Mode selectivity in reactions of H with $\text{HOD}(100)$, $\text{HOD}(001)$, and $\text{HOD}(002)$. Journal of Chemical Physics, 1992, 96, 7852-7854.	3.0	90
52	Three-State Trajectory Surface Hopping Studies of the Photodissociation Dynamics of Formaldehyde on <i>ab Initio</i> Potential Energy Surfaces. Journal of the American Chemical Society, 2011, 133, 7957-7968.	13.7	90
53	Experimental and reduced dimensionality quantum rate coefficients for $\text{H}_2(\text{D}_2)+\text{CN} \rightarrow \text{H}(\text{D})\text{CN}+\text{H}(\text{D})$. Journal of Chemical Physics, 1990, 93, 4730-4739.	3.0	89
54	Variational calculations of rovibrational energies of CH_4 and isotopomers in full dimensionality using an <i>ab initio</i> potential. Journal of Chemical Physics, 1999, 110, 8417-8423.	3.0	89

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55	A wave-packet calculation of the effect of reactant rotation and alignment on product branching in the $\text{O}(1\text{D})+\text{HCl} \rightarrow \text{ClO}+\text{H}$, $\text{OH}+\text{Cl}$ reactions. <i>Journal of Chemical Physics</i> , 2000, 113, 1-3.	3.0	89
56	Quasiclassical Trajectory Calculations of Acetaldehyde Dissociation on a Global Potential Energy Surface Indicate Significant Non-transition State Dynamics. <i>Journal of Physical Chemistry A</i> , 2007, 111, 8282-8285.	2.5	89
57	Experimental and Theoretical Investigations of Energy Transfer and Hydrogen-Bond Breaking in the Water Dimer. <i>Journal of the American Chemical Society</i> , 2012, 134, 15430-15435.	13.7	89
58	$\hat{\text{I}}^{\text{r}}$ -machine learning for potential energy surfaces: A PIP approach to bring a DFT-based PES to CCSD(T) level of theory. <i>Journal of Chemical Physics</i> , 2021, 154, 051102.	3.0	89
59	Ab Initio Diffusion Monte Carlo Calculations of the Quantum Behavior of CH_5^+ in Full Dimensionality. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4991-4994.	2.5	87
60	Mode Selectivity for a $\text{O}(\text{P}) + \text{CH}_4 \rightarrow \text{OH} + \text{CH}_3$ Reaction on an Ab Initio Potential Energy Surface. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 3776-3780.	4.6	87
61	High-Level, First-Principles, Full-Dimensional Quantum Calculation of the Ro-vibrational Spectrum of the Simplest Criegee Intermediate (CH_2OO). <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2364-2369.	4.6	86
62	CH_3CHO Roaming Dynamics in CH_3CHO Photodissociation Revealed on a Global Potential Energy Surface. <i>Journal of Physical Chemistry A</i> , 2008, 112, 9344-9351.	2.5	84
63	A theoretical study of the vibrational energy spectrum of the HOCl/HClO system on an accurate ab initio potential energy surface. <i>Journal of Chemical Physics</i> , 1999, 111, 7446-7456.	3.0	83
64	The roaming atom pathway in formaldehyde decomposition. <i>Journal of Chemical Physics</i> , 2006, 125, 044303.	3.0	83
65	Structure, Anharmonic Vibrational Frequencies, and Intensities of NNHNN^+ . <i>Journal of Physical Chemistry A</i> , 2015, 119, 11623-11631.	2.5	81
66	Complex coordinate calculations of Feshbach resonance energies and widths for a collinear triatomic system. <i>Journal of Chemical Physics</i> , 1983, 78, 3952-3958.	3.0	80
67	A theoretical study of vibrational mode coupling in H_2O_2^+ . <i>Journal of Chemical Physics</i> , 2003, 119, 6571-6580.	3.0	79
68	Assessing Gaussian Process Regression and Permutationally Invariant Polynomial Approaches To Represent High-Dimensional Potential Energy Surfaces. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3381-3396.	5.3	78
69	Reduced dimensionality quantum calculations of mode specificity in $\text{OH}+\text{H}_2 \rightarrow \text{H}_2\text{O}+\text{H}$. <i>Journal of Chemical Physics</i> , 1992, 96, 8906-8913.	3.0	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 4-mode subspaces. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 24835-24840.	2.8	76
71	Sudden rotation calculations of atom-molecule scattering. <i>Journal of Chemical Physics</i> , 1977, 66, 288-295.	3.0	75
72	Roaming reactions: The third way. <i>Physics Today</i> , 2011, 64, 33-37.	0.3	75

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73	L2 calculations of resonances and final rotational distributions for $\text{HCO}^+\text{H}+\text{CO}$. Journal of Chemical Physics, 1994, 100, 1021-1027.	3.0	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.	3.0	74
75	Infrared identification of the Criegee intermediates syn- and anti- CH_3CHOO , and their distinct conformation-dependent reactivity. Nature Communications, 2015, 6, 7012.	12.8	74
76	A simple method to adjust potential energy surfaces: Application to HCO . Journal of Chemical Physics, 1991, 94, 816-817.	3.0	71
77	New insights on reaction dynamics from formaldehyde photodissociation. Physical Chemistry Chemical Physics, 2006, 8, 321-332.	2.8	69
78	Differences in the Vibrational Dynamics of H_2O and D_2O : Observation of Symmetric and Antisymmetric Stretching Vibrations in Heavy Water. Journal of Physical Chemistry Letters, 2016, 7, 1769-1774.	4.6	68
79	Coupled channel calculation of resonances in $\text{H}+\text{CO}$. Journal of Chemical Physics, 1986, 84, 4888-4893.	3.0	67
80	Full-dimensionality quantum calculations of acetylene-vinylidene isomerization. Journal of Chemical Physics, 2003, 118, 10012-10023.	3.0	67
81	Signatures of H_2CO Photodissociation from Two Electronic States. Science, 2006, 311, 1443-1446.	12.6	67
82	Theories and simulations of roaming. Chemical Society Reviews, 2017, 46, 7615-7624.	38.1	67
83	Resonances: A Bridge between Spectroscopy and Dynamics. Journal of Physical Chemistry A, 1998, 102, 3006-3017.	2.5	65
84	Directab initio variational calculation of vibrational energies of the $\text{H}_2\text{O}\cdots\text{Cl}^-$ complex and resolution of experimental differences. Journal of Chemical Physics, 2000, 113, 8401-8403.	3.0	64
85	Quasiclassical trajectory study of formaldehyde unimolecular dissociation: $\text{H}_2\text{CO}^+\text{H}_2+\text{CO}$, $\text{H}+\text{HCO}$. Journal of Chemical Physics, 2005, 122, 114313.	3.0	63
86	An adjusted global potential surface for HCN based on rigorous vibrational calculations. Journal of Chemical Physics, 1991, 95, 6309-6316.	3.0	62
87	Calculations of rovibrational energies and dipole transition intensities for polyatomic molecules using <code>MULTIMODE</code> . Journal of Chemical Physics, 2009, 131, 224106.	3.0	62
88	Roaming Pathway Leading to Unexpected Water + Vinyl Products in $\text{C}_2\text{H}_4\text{OH}$ Dissociation. Journal of Physical Chemistry Letters, 2010, 1, 3058-3065.	4.6	62
89	Quantum calculations of mode specificity in reactions of H with HOD and H_2O . Journal of Chemical Physics, 1993, 98, 6235-6247.	3.0	61
90	Ab initio potential energy surface and rovibrational energies of H_3O^+ and its isotopomers. Journal of Chemical Physics, 2003, 118, 5431-5441.	3.0	61

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91	Vibrational Levels of Methanol Calculated by the Reaction Path Version of MULTIMODE, Using an ab initio, Full-Dimensional Potential. Journal of Physical Chemistry A, 2007, 111, 7317-7321.	2.5	61
92	Quantum dynamics of CO+H ₂ in full dimensionality. Nature Communications, 2015, 6, 6629.	12.8	61
93	Capturing roaming molecular fragments in real time. Science, 2020, 370, 1072-1077.	12.6	61
94	Permutationally Invariant Fitting of Many-Body, Non-covalent Interactions with Application to Three-Body Methane+Water. Journal of Chemical Theory and Computation, 2015, 11, 1631-1638.	5.3	60
95	Resonances in the O(3P)+HCl reaction due to van der Waals minima. Journal of Chemical Physics, 2002, 116, 7461-7467.	3.0	59
96	Overview of reduced dimensionality quantum approaches to reactive scattering. Theoretical Chemistry Accounts, 2002, 108, 125-133.	1.4	59
97	A comparative study of the reaction dynamics of several potential energy surfaces of O(3P)+H ₂ +OH+H. I. Journal of Chemical Physics, 1981, 74, 4984-4996.	3.0	58
98	Argon Predissociation Spectroscopy of the OH-H ₂ O and Cl-H ₂ O Complexes in the 1000-1900 cm ⁻¹ Region: Intramolecular Bending Transitions and the Search for the Shared-Proton Fundamental in the Hydroxide Monohydrate. Journal of Physical Chemistry A, 2005, 109, 571-575.	2.5	56
99	Communication: VSCF/VCi vibrational spectroscopy of H ₂ O ₃ ⁺ and H ₂ O ₄ ⁺ using high-level, many-body potential energy surface and dipole moment surfaces. Journal of Chemical Physics, 2017, 146, 121102.	3.0	56
100	A three-dimensional L2 simulation of the photodetachment spectra of ClHCl ⁺ and IHI ⁺ . Journal of Chemical Physics, 1989, 91, 4615-4624.	3.0	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.	2.6	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.	4.6	55
103	Quasiclassical Trajectory Study of CH ₃ NO ₂ Decomposition via Roaming Mediated Isomerization Using a Global Potential Energy Surface. Journal of Physical Chemistry A, 2013, 117, 11665-11672.	2.5	54
104	Plug and play full-dimensional ab initio potential energy and dipole moment surfaces and anharmonic vibrational analysis for CH ₄ +H ₂ O. Physical Chemistry Chemical Physics, 2015, 17, 8172-8181.	2.8	54
105	Energy dependence of the roaming atom pathway in formaldehyde decomposition. Journal of Chemical Physics, 2007, 126, 044314.	3.0	53
106	The internal coordinate path Hamiltonian; application to methanol and malonaldehyde. Molecular Physics, 2003, 101, 3513-3525.	1.7	51
107	Reaction dynamics for O(3P)+H ₂ and D ₂ . IV. Reduced dimensionality quantum and quasiclassical rate constants with an adiabatic incorporation of the bending motion. Journal of Chemical Physics, 1984, 81, 1739-1752.	3.0	49
108	Quasiclassical trajectory study of the postquenching dynamics of OH+H ₂ by H ₂ /D ₂ on a global potential energy surface. Journal of Chemical Physics, 2010, 133, 164306.	3.0	49

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109	Crossed Molecular Beams and Quasiclassical Trajectory Surface Hopping Studies of the Multichannel Nonadiabatic $O(^3P) + \text{Ethylene}$ Reaction at High Collision Energy. <i>Journal of Physical Chemistry A</i> , 2015, 119, 12498-12511.	2.5	49
110	Energetics and Predissociation Dynamics of Small Water, HCl, and Mixed HCl–Water Clusters. <i>Chemical Reviews</i> , 2016, 116, 4913-4936.	47.7	49
111	The infrared spectrum of the hydrogen bifluoride anion: unprecedented variation with level of theory. <i>Chemical Physics Letters</i> , 1986, 131, 352-358.	2.6	48
112	A comparative study of the reaction dynamics of several potential energy surfaces for $O(3P) + H_2 \rightarrow OH + H$. II. Collinear exact quantum and quasiclassical reaction probabilities. <i>Journal of Chemical Physics</i> , 1982, 76, 3563-3582.	3.0	47
113	The effect of rotation on resonances: Application to HCO. <i>Journal of Chemical Physics</i> , 1996, 105, 9884-9889.	3.0	47
114	Photodissociation dynamics of nitromethane and methyl nitrite by infrared multiphoton dissociation imaging with quasiclassical trajectory calculations: Signatures of the roaming pathway. <i>Journal of Chemical Physics</i> , 2014, 140, 054305.	3.0	47
115	Three Reaction Pathways in the $H + HCO \rightarrow H_2 + CO$ Reaction. <i>Journal of Physical Chemistry A</i> , 2009, 113, 4138-4144.	2.5	46
116	Coupled-monomers in molecular assemblies: Theory and application to the water tetramer, pentamer, and ring hexamer. <i>Journal of Chemical Physics</i> , 2012, 136, 144113.	3.0	46
117	Experimental and Theoretical Investigations of the Dissociation Energy (D_0) and Dynamics of the Water Trimer, $(H_2O)_3$. <i>Journal of Physical Chemistry A</i> , 2013, 117, 7207-7216.	2.5	46
118	Experimental and Theoretical Investigations of Energy Transfer and Hydrogen-Bond Breaking in Small Water and HCl Clusters. <i>Accounts of Chemical Research</i> , 2014, 47, 2700-2709.	15.6	46
119	Quantum calculations of the IR spectrum of liquid water using <i>ab initio</i> and model potential and dipole moment surfaces and comparison with experiment. <i>Journal of Chemical Physics</i> , 2015, 142, 194502.	3.0	46
120	Vibrational analysis of HOCl up to 98% of the dissociation energy with a Fermi resonance Hamiltonian. <i>Journal of Chemical Physics</i> , 1999, 111, 6807-6820.	3.0	45
121	Roaming Under the Microscope: Trajectory Study of Formaldehyde Dissociation. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5103-5114.	2.5	45
122	The calculated infrared spectrum of $Cl^- \cdots H_2O$ using a new full dimensional <i>ab initio</i> potential surface and dipole moment surface. <i>Journal of Chemical Physics</i> , 2006, 125, 133206.	3.0	44
123	Are Roaming and Conventional Saddle Points for H_2CO and CH_3CHO Dissociation to Molecular Products Isolated from Each Other?. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 834-838.	4.6	44
124	Mode-specific tunneling using the <i>Q</i> path: Theory and an application to full-dimensional malonaldehyde. <i>Journal of Chemical Physics</i> , 2013, 139, 154303.	3.0	44
125	Disentangling the Complex Vibrational Spectrum of the Protonated Water Trimer, $H^+(H_2O)_3$, with Two-Color IR-IR Photodissociation of the Bare Ion and Anharmonic VSCF/VCI Theory. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3782-3789.	4.6	44
126	Quantum and classical dynamics of a coupled double well oscillator. <i>Journal of Chemical Physics</i> , 1981, 74, 5057-5075.	3.0	43

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127	High-Level Quantum Calculations of the IR Spectra of the Eigen, Zundel, and Ring Isomers of $\text{H}^+ \cdot (\text{H}_2\text{O})_4$ Find a Single Match to Experiment. Journal of the American Chemical Society, 2017, 139, 10984-10987.	13.7	43
128	Using Gradients in Permutationally Invariant Polynomial Potential Fitting: A Demonstration for CH_4 Using as Few as 100 Configurations. Journal of Chemical Theory and Computation, 2019, 15, 2826-2835.	5.3	43
129	Quasiclassical trajectory studies of rigid rotor-rigid surface scattering. I. Flat surface. Journal of Chemical Physics, 1982, 77, 5441-5449.	3.0	42
130	Quantum calculations of the rate constant for the $\text{O}(3\text{P}) + \text{HCl}$ reaction on new ab initio $3\text{A}''^3$ and $3\text{A}''^2$ surfaces. Journal of Chemical Physics, 2003, 119, 9601-9608.	3.0	42
131	Communication: Spectroscopic consequences of proton delocalization in OCHCO^+ . Journal of Chemical Physics, 2015, 143, 071102.	3.0	42
132	A Machine Learning Approach for Prediction of Rate Constants. Journal of Physical Chemistry Letters, 2019, 10, 5250-5258.	4.6	42
133	New approximate quantum cross sections for the $\text{H} + \text{H}_2$ reaction. Journal of Chemical Physics, 1981, 75, 5199-5201.	3.0	41
134	A comparative study of the reaction dynamics of the $\text{O}(3\text{P}) + \text{H}_2\text{O}^+ \rightarrow \text{OH} + \text{H}$ 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.	3.0	41
135	Theoretical studies of the reactivity and spectroscopy of $\text{H} + \text{CO} = \text{HCO}$. I. Stabilization and scattering studies of resonances for $J=0$ on the Harding ab initio surface. Journal of Chemical Physics, 1992, 96, 2799-2811.	3.0	41
136	Mid- and Far-IR Spectra of H_5^+ and D_5^+ Compared to the Predictions of Anharmonic Theory. Journal of Physical Chemistry Letters, 2012, 3, 3160-3166.	4.6	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.	4.6	41
138	One-dimensional tunneling calculations in the imaginary-frequency, rectilinear saddle-point normal mode. Journal of Chemical Physics, 2008, 129, 121103.	3.0	40
139	Evidence for Vinylidene Production in the Photodissociation of the Allyl Radical. Journal of Physical Chemistry Letters, 2010, 1, 1875-1880.	4.6	40
140	Quasiclassical Trajectory Calculations of the Dissociation Dynamics of CH_3CHO at High Energy Yield Many Products. Journal of Physical Chemistry Letters, 2011, 2, 1715-1719.	4.6	40
141	Full-dimensional, high-level <i>ab initio</i> potential energy surfaces for $\text{H}_2(\text{H}_2\text{O})$ and $\text{H}_2(\text{H}_2\text{O})_2$ with application to hydrogen clathrate hydrates. Journal of Chemical Physics, 2015, 143, 084302.	3.0	40
142	Normal-mode analysis without the Hessian: A driven molecular-dynamics approach. Journal of Chemical Physics, 2003, 119, 646-650.	3.0	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.	3.0	39
144	Benchmark Electronic Structure Calculations for $\text{H}_3\text{O}^+ \cdot (\text{H}_2\text{O})_n$, $n = 0-5$, 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.	5.3	39

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145	Breaking the Coupled Cluster Barrier for Machine-Learned Potentials of Large Molecules: The Case of 15-Atom Acetylacetone. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 4902-4909.	4.6	39
146	A movable basis method to calculate vibrational energies of molecules. <i>Journal of Chemical Physics</i> , 1990, 93, 1774-1784.	3.0	38
147	Quantum calculations of unusual mode specificity in $H+C_2H_2 \rightarrow H_2+C_2H$. <i>Journal of Chemical Physics</i> , 1994, 101, 8646-8662.	3.0	38
148	Skirting the transition state, a new paradigm in reaction rate theory. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 16061-16062.	7.1	38
149	Deconstructing Prominent Bands in the Terahertz Spectra of $H_2O_3^+$ and $H_2O_4^+$: Intermolecular Modes in Eigen Clusters. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 798-803.	4.6	38
150	Recovering a full dimensional quantum rate constant from a reduced dimensionality calculation: Application to the $OH+CO \rightarrow H+CO_2$ reaction. <i>Journal of Chemical Physics</i> , 1996, 105, 2280-2286.	3.0	37
151	Full dimensionality quantum calculations of acetylene/vinylidene isomerization. <i>Journal of Chemical Physics</i> , 2002, 117, 5507-5510.	3.0	37
152	Ab Initio Potential Energy Surface and Vibrational Energies of H_3O^+ and Its Isotopomers. <i>Journal of Physical Chemistry B</i> , 2002, 106, 8182-8188.	2.6	37
153	Communication: A benchmark-quality, full-dimensional <i>ab initio</i> potential energy surface for Ar-HOCO. <i>Journal of Chemical Physics</i> , 2014, 140, .	3.0	37
154	A fragmented, permutationally invariant polynomial approach for potential energy surfaces of large molecules: Application to <i>N</i> -methyl acetamide. <i>Journal of Chemical Physics</i> , 2019, 150, 141101.	3.0	37
155	Vibrational dynamics up to the dissociation threshold: A case study of two-dimensional HOCl. <i>Journal of Chemical Physics</i> , 2000, 113, 9610-9621.	3.0	36
156	Quantum Calculations of Intramolecular IR Spectra of Ice Models Using Ab Initio Potential and Dipole Moment Surfaces. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 3671-3676.	4.6	36
157	Quantum approaches to vibrational dynamics and spectroscopy: is ease of interpretation sacrificed as rigor increases?. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 3397-3413.	2.8	35
158	Quasiclassical studies of rigid rotor-surface diffraction scattering. <i>Journal of Chemical Physics</i> , 1977, 66, 1122-1126.	3.0	34
159	Perturbative inversion of the HOCl potential energy surface via singular value decomposition. <i>Chemical Physics Letters</i> , 1999, 312, 494-502.	2.6	34
160	CHEMISTRY: Beyond Platonic Molecules. <i>Science</i> , 2000, 290, 724-725.	12.6	34
161	The determination of molecular properties from MULTIMODE with an application to the calculation of Franck-Condon factors for photoionization of CF_3 . <i>Molecular Physics</i> , 2006, 104, 33-45.	1.7	34
162	Photodissociation Dynamics of Formaldehyde Initiated at the T_{1/S_0} Minimum Energy Crossing Configurations. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13267-13270.	2.5	34

#	ARTICLE	IF	CITATIONS
163	Classical, Thermostated Ring Polymer, and Quantum VSCF/VCI Calculations of IR Spectra of $\text{H}_{7+3}\text{O}_{3+4}$ and $\text{H}_{9+4}\text{O}_{4+4}$ (Eigen) and Comparison with Experiment. Journal of Physical Chemistry A, 2019, 123, 1399-1409.	2.5	34
164	Theoretical stabilization and scattering studies of resonances in the addition reaction $\text{H}+\text{CO}=\text{HCO}$. Journal of Chemical Physics, 1991, 94, 4192-4194.	3.0	33
165	Quasiclassical trajectory calculations of photodissociation of $\text{ArH}_2\text{O}(\text{X}^1\text{f}^1\text{A}^1)$ and $\text{H}_2\text{O}(\text{X}^1\text{f}^1\text{A}^1)$. Journal of Chemical Physics, 1996, 104, 8348-8356.	3.0	33
166	“Spectator” modes in resonance-driven reactions: Three-dimensional quantum calculations of HOCO resonances. Journal of Chemical Physics, 1998, 108, 511-518.	3.0	33
167	Normal mode analysis using the driven molecular dynamics method. II. An application to biological macromolecules. Journal of Chemical Physics, 2004, 121, 5646-5653.	3.0	33
168	Proton affinity and enthalpy of formation of formaldehyde. International Journal of Quantum Chemistry, 2009, 109, 2393-2409.	2.0	33
169	Quasiclassical Trajectory Calculations of the Rate Constant of the $\text{OH} + \text{HBr} \rightarrow \text{Br} + \text{H}_2\text{O}$ Reaction Using a Full-Dimensional Ab Initio Potential Energy Surface Over the Temperature Range 5 to 500 K. Journal of Physical Chemistry Letters, 2014, 5, 706-712.	4.6	33
170	A new (multi-reference configuration interaction) potential energy surface for H_2CO and preliminary studies of roaming. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2017, 375, 20160194.	3.4	33
171	Efficient Generation of Permutationally Invariant Potential Energy Surfaces for Large Molecules. Journal of Chemical Theory and Computation, 2020, 16, 3264-3272.	5.3	33
172	Translational energy dependence of the $\text{Cl}+\text{CH}_4(\text{v}_1=0, \text{v}_2=1)$ reactions: a joint crossed-beam and quasiclassical trajectory study. Molecular Physics, 2012, 110, 1617-1626.	1.7	32
173	Full-dimensional quantum dynamics of CO in collision with H ₂ . Journal of Chemical Physics, 2016, 145, 034308.	3.0	32
174	Full and fragmented permutationally invariant polynomial potential energy surfaces for <i>trans</i> - and <i>cis</i> -N-methyl acetamide and isomerization saddle points. Journal of Chemical Physics, 2019, 151, 084306.	3.0	32
175	Sudden approximation calculations of reactive scattering: The $\text{H}+\text{H}_2$ reaction. Journal of Chemical Physics, 1978, 68, 3940-3941.	3.0	31
176	A comparative study of the quantum dynamics and rate constants of the $\text{O}(3\text{P})+\text{HCl}$ reaction described by two potential surfaces. Journal of Chemical Physics, 2000, 113, 227-236.	3.0	31
177	Multimode calculations of rovibrational energies of C_2H_4 and C_2D_4 . Molecular Physics, 2012, 110, 775-781.	1.7	31
178	Transferable ab Initio Dipole Moment for Water: Three Applications to Bulk Water. Journal of Physical Chemistry B, 2016, 120, 1735-1742.	2.6	31
179	Rotational distributions and collision lifetimes in $\text{H}+\text{CO}$ scattering. Journal of Chemical Physics, 1986, 85, 6225-6226.	3.0	30
180	Full dimensional calculations of vibrational energies of H_3O^+ and D_3O^+ . Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 839-848.	3.9	30

#	ARTICLE	IF	CITATIONS
181	Dipole Surface and Infrared Intensities for the <i>cis</i> - and <i>trans</i> -HOCO and DOCO Radicals. Journal of Physical Chemistry A, 2013, 117, 6932-6939.	2.5	30
182	Ab Initio Potential for $H_3O^+ \hat{+} H^+ + H_2O$: A Step to a Many-Body Representation of the Hydrated Proton?. Journal of Chemical Theory and Computation, 2016, 12, 5284-5292.	5.3	30
183	Revisiting Adiabatic Switching for Initial Conditions in Quasi-Classical Trajectory Calculations: Application to CH_4 . Journal of Physical Chemistry A, 2016, 120, 4988-4993.	2.5	30
184	Investigations of transformed mass-scaled Jacobi coordinates for vibrations of polyatomic molecules with application to H ₂ O. Journal of Chemical Physics, 1989, 90, 2708-2713.	3.0	29
185	Reduced dimensionality quantum calculations of acetylene vinylidene isomerization. Journal of Chemical Physics, 2002, 116, 6667-6673.	3.0	29
186	Inverse perturbation via singular value decomposition: Application to correction of potential surface for HCN. Journal of Chemical Physics, 1997, 107, 3602-3610.	3.0	28
187	Full Dimensional Quantum Calculations of Vibrational Energies of N-Methyl Acetamide. Journal of Physical Chemistry A, 2007, 111, 5593-5598.	2.5	28
188	Comparison of quantum, classical, and ring-polymer molecular dynamics infra-red spectra of $Cl_2^+(H_2O)$ and $H^+(H_2O)_2$. Chemical Physics Letters, 2008, 450, 253-257.	2.6	28
189	Classical Trajectory Study of Energy Transfer in Collisions of Highly Excited Allyl Radical with Argon. Journal of Physical Chemistry A, 2013, 117, 14028-14041.	2.5	28
190	Chemical Activation through Super Energy Transfer Collisions. Journal of the American Chemical Society, 2014, 136, 1682-1685.	13.7	28
191	Isolating the spectral signature of H_3O^+ in the smallest droplet of dissociated HCl acid. Physical Chemistry Chemical Physics, 2015, 17, 6222-6226.	2.8	28
192	A Machine Learning Approach for Rate Constants. II. Clustering, Training, and Predictions for the $O(^3P) + HCl \hat{+} OH + Cl$ Reaction. Journal of Physical Chemistry A, 2020, 124, 5746-5755.	2.5	28
193	Collision-induced and complex-mediated roaming dynamics in the $H + C_2H_4 \hat{+} H_2 + C_2H_3$ reaction. Chemical Science, 2020, 11, 2148-2154.	7.4	28
194	Quasitrapping and rainbow mechanisms in model rigid-rotor rigid-surface scattering. Journal of Chemical Physics, 1982, 76, 1168-1170.	3.0	27
195	Reaction dynamics for $O(^3P) + HD$. V. Reduced dimensionality quantum and quasiclassical reaction probabilities and rate constants with an adiabatic incorporation of the bending motion. Journal of Chemical Physics, 1987, 86, 1967-1975.	3.0	27
196	Quantum scattering calculations of energy transfer and dissociation of HCO in collisions with Ar. Journal of Chemical Physics, 1995, 103, 9661-9668.	3.0	27
197	Variation of the resonance width of $HOCl(6\frac{1}{2}OH)$ with total angular momentum: Comparison between <i>ab initio</i> , theory and experiment. Journal of Chemical Physics, 1999, 110, 9789-9792.	3.0	27
198	Nonseparable transition state theory for nonzero total angular momentum: Implications for J shifting and application to the $OH + H_2$ reaction. Journal of Chemical Physics, 1999, 110, 4428-4434.	3.0	27

#	ARTICLE	IF	CITATIONS
199	Effects of Zero-Point Delocalization on the Vibrational Frequencies of Mixed HCl and Water Clusters. Journal of Physical Chemistry Letters, 2014, 5, 2247-2253.	4.6	27
200	Ab Initio Quantum Approaches to the IR Spectroscopy of Water and Hydrates. Journal of Physical Chemistry Letters, 2015, 6, 366-373.	4.6	27
201	Tag-Free and Isotopomer-Selective Vibrational Spectroscopy of the Cryogenically Cooled H_9O_4^+ Cation with Two-Color, IR-IR Double-Resonance Photoexcitation: Isolating the Spectral Signature of a Single OH Group in the Hydronium Ion Core. Journal of Physical Chemistry A, 2018, 122, 9275-9284.	2.5	27
202	Direct diabaticization and analytic representation of coupled potential energy surfaces and couplings for the reactive quenching of the excited $2^1\Sigma^+$ state of OH by molecular hydrogen. Journal of Chemical Physics, 2019, 151, 104311.	3.0	27
203	Permutationally invariant polynomial potential energy surfaces for tropolone and H and D atom tunneling dynamics. Journal of Chemical Physics, 2020, 153, 024107.	3.0	27
204	Tests of collinear quasiclassical trajectory transmission coefficient correction to transition state theory. Journal of Chemical Physics, 1981, 75, 141-147.	3.0	26
205	New vibrational self-consistent field program for large molecules. Journal of Computational Chemistry, 1996, 17, 1645-1652.	3.3	26
206	Formaldehyde photodissociation: Dependence on total angular momentum and rotational alignment of the CO product. Journal of Chemical Physics, 2007, 126, 134305.	3.0	26
207	Pruning the Hamiltonian Matrix in MULTIMODE: Test for C_2H_4 and Application to CH_3NO_2 Using a New Ab Initio Potential Energy Surface. Journal of Physical Chemistry A, 2015, 119, 11632-11640.	2.5	26
208	Full-dimensional quantum dynamics of rovibrationally inelastic scattering between CN and H_2 . Journal of Chemical Physics, 2016, 145, 224307.	3.0	26
209	Quantum Calculation of the Recombination Rate Constant of $\text{H} + \text{CO} \rightarrow \text{HCO}$. The Journal of Physical Chemistry, 1996, 100, 15165-15170.	2.9	25
210	Quantum Local Monomer IR Spectrum of Liquid D_2O at 300 K from 0 to 4000 cm^{-1} Is in Near-Quantitative Agreement with Experiment. Journal of Physical Chemistry B, 2016, 120, 2824-2828.	2.6	25
211	Full-Dimensional Quantum Dynamics of SiO in Collision with H_2 . Journal of Physical Chemistry A, 2018, 122, 1511-1520.	2.5	25
212	Observation of the Low-Frequency Spectrum of the Water Dimer as a Sensitive Test of the Water Dimer Potential and Dipole Moment Surfaces. Angewandte Chemie - International Edition, 2019, 58, 13119-13126.	13.8	25
213	A CCSD(T)-Based 4-Body Potential for Water. Journal of Physical Chemistry Letters, 2021, 12, 10318-10324.	4.6	25
214	Sudden rotation total rotational inelastic cross sections for $4\text{He} + \text{I}_2^*$. Journal of Chemical Physics, 1977, 66, 296-297.	3.0	24
215	Quantum calculations of the effect of bend excitation in methane on the HCl rotational distribution in the reaction $\text{CH}_4 + \text{Cl} \rightarrow \text{CH}_3 + \text{HCl}$. Journal of Chemical Physics, 2000, 113, 4495-4497.	3.0	24
216	A novel Gaussian Binning (1GB) analysis of vibrational state distributions in highly excited mH_2O from reactive quenching of OH^* by mH_2 . Journal of Chemical Physics, 2013, 139, 044104.	3.0	24

#	ARTICLE	IF	CITATIONS
217	Zero-point Energy is Needed in Molecular Dynamics Calculations to Access the Saddle Point for $\text{H}+\text{HCN}\hat{\dagger}\text{H}<\sub>2</sub>\text{CN}^*$ and $<i>\text{cis/trans}</i>\text{HCNH}^*$ on a New Potential Energy Surface. Journal of Chemical Theory and Computation, 2013, 9, 901-908.	5.3	24
218	Two-component, $<i>\text{ab initio}</i>$ potential energy surface for $\text{CO}_2\hat{\dagger}\text{H}_2\text{O}$, extension to the hydrate clathrate, $\text{CO}_2@(\text{H}_2\text{O})_{20}$, and VSCF/VCI vibrational analyses of both. Journal of Chemical Physics, 2017, 147, 161714.	3.0	24
219	Energy transfer between vibrationally excited carbon monoxide based on a highly accurate six-dimensional potential energy surface. Journal of Chemical Physics, 2020, 153, 054310.	3.0	24
220	Rotational resonances in the $\text{H}<\sub>2</sub>\text{CO}$ roaming reaction are revealed by detailed correlations. Science, 2020, 369, 1592-1596.	12.6	24
221	Full-dimensional potential energy surface for acetylacetone and tunneling splittings. Physical Chemistry Chemical Physics, 2021, 23, 7758-7767.	2.8	24
222	Permutationally invariant polynomial regression for energies and gradients, using reverse differentiation, achieves orders of magnitude speed-up with high precision compared to other machine learning methods. Journal of Chemical Physics, 2022, 156, 044120.	3.0	24
223	Thermal and State-Selected Rate Coefficients for the $\text{O}(3\text{P}) + \text{HCl}$ Reaction and New Calculations of the Barrier Height and Width. Journal of Physical Chemistry A, 2001, 105, 2298-2307.	2.5	23
224	Quantum vibrational analysis and infrared spectra of microhydrated sodium ions using an $<i>\text{ab initio}</i>$ potential. Journal of Chemical Physics, 2011, 134, 114311.	3.0	23
225	Quasiclassical Trajectory Studies of the Photodissociation Dynamics of $\text{NO}<\sub>3</sub>$ from the $\text{D}<\sub>0</sub>$ and $\text{D}<\sub>1</sub>$ Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2013, 9, 893-900.	5.3	23
226	High-dimensional fitting of sparse datasets of CCSD(T) electronic energies and MP2 dipole moments, illustrated for the formic acid dimer and its complex IR spectrum. Journal of Chemical Physics, 2018, 148, 241713.	3.0	23
227	High-Level VSCF/VCI Calculations Decode the Vibrational Spectrum of the Aqueous Proton. Journal of Physical Chemistry B, 2019, 123, 7214-7224.	2.6	23
228	Tracking Hydronium/Water Stretches in Magic $\text{H}<\sub>3</sub>\text{O}<\sup>+</sup>(\text{H}<\sub>2</sub>\text{O})<\sub>20</sub>$ Clusters through High-level Quantum VSCF/VCI Calculations. Journal of Physical Chemistry A, 2020, 124, 1167-1175.	2.5	23
229	Full-dimensional, $<i>\text{ab initio}</i>$ potential energy surface for glycine with characterization of stationary points and zero-point energy calculations by means of diffusion Monte Carlo and semiclassical dynamics. Journal of Chemical Physics, 2020, 153, 244301.	3.0	23
230	Reduced dimensionality diatom $\hat{\dagger}$ diatom reactive scattering: Application to a model $\text{H}_2+\text{A}_2\hat{\dagger}\text{H}+\text{HA}_2$ reaction. Journal of Chemical Physics, 1990, 92, 1021-1029.	3.0	22
231	"Morphing" of ab initio-based interaction potentials to spectroscopic accuracy: Application to $\text{Cl}(\text{H}_2\text{O})$. Pure and Applied Chemistry, 2004, 76, 29-35.	1.9	22
232	Reduced-Dimensional Quantum Approach to Tunneling Splittings Using Saddle-Point Normal Coordinates. Journal of Physical Chemistry A, 2009, 113, 7556-7562.	2.5	22
233	Variational Calculations of Vibrational Energies and IR Spectra of $<i>\text{trans}</i>$ - and $<i>\text{cis}</i>$ -HOCO Using New ab Initio Potential Energy and Dipole Moment Surfaces. Journal of Physical Chemistry A, 2013, 117, 9343-9352.	2.5	22
234	Photodissociation of $\text{CH}<\sub>3</sub>\text{CHO}$ at 248 nm: identification of the channels of roaming, triple fragmentation and the transition state. Physical Chemistry Chemical Physics, 2017, 19, 18628-18634.	2.8	22

#	ARTICLE	IF	CITATIONS
235	IR Spectra of (HCOOH) ₂ and (DCOOH) ₂ : Experiment, VSCF/VCI, and Ab Initio Molecular Dynamics Calculations Using Full-Dimensional Potential and Dipole Moment Surfaces. Journal of Physical Chemistry Letters, 2018, 9, 2604-2610.	4.6	22
236	Application of adiabatic switching to vibrational energies of three-dimensional HCO, H ₂ O, and H ₂ CO. Journal of Chemical Physics, 1988, 89, 3124-3130.	3.0	21
237	Time dependence of OH overtone relaxation in the hydroperoxyl radical. Journal of Chemical Physics, 1992, 96, 1919-1930.	3.0	21
238	Potential energy surface and vibrational eigenstates of the H ₂ –CN(X ² Σ ⁺) van der Waals complex. Journal of Chemical Physics, 1999, 110, 10380-10392.	3.0	21
239	High torsional vibrational energies of H ₂ O ₂ and CH ₃ OH studied by MULTIMODE with a large amplitude motion coupled to two effective contraction schemes. Molecular Physics, 2009, 107, 727-737.	1.7	21
240	Multimode calculations of rovibrational energies and dipole transition intensities for polyatomic molecules with torsional motion: Application to H ₂ O ₂ . Journal of Chemical Physics, 2011, 135, 014308.	3.0	21
241	Reduced Dimensionality Theories of Quantum Reactive Scattering: Applications to Mu+H ₂ , H+H ₂ , O(3P)+H ₂ , D ₂ and HD. , 1986, , 47-76.		20
242	Application of complex L ₂ functions to the calculation of photodissociation processes. Journal of Chemical Physics, 1994, 100, 7229-7238.	3.0	20
243	On using potential, gradient, and Hessian data in least squares fits of potentials: Application and tests for H ₂ O. Journal of Chemical Physics, 2002, 117, 10487-10492.	3.0	20
244	Local-Monomer Calculations of the Intramolecular IR Spectra of the Cage and Prism Isomers of HOD(D ₂ O) ₅ and HOD and D ₂ O Ice Ih. Journal of Physical Chemistry B, 2014, 118, 14124-14131.	2.6	20
245	Quasiclassical Trajectory Calculations of the N(² D) + H ₂ O Reaction Elucidating the Formation Mechanism of HNO and HON Seen in Molecular Beam Experiments. Journal of Physical Chemistry Letters, 2014, 5, 3508-3513.	4.6	20
246	Ab initio potential energy and dipole moment surfaces of the F ⁺ (H ₂ O) complex. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 119, 59-62.	3.9	20
247	How the Zundel (H ₅ O ₂ ⁺) Potential Can Be Used to Predict the Proton Stretch and Bend Frequencies of Larger Protonated Water Clusters. Journal of Physical Chemistry Letters, 2016, 7, 5259-5265.	4.6	20
248	Formaldehyde roaming dynamics: Comparison of quasi-classical trajectory calculations and experiments. Journal of Chemical Physics, 2017, 147, 013936.	3.0	20
249	Decoding the 2D IR spectrum of the aqueous proton with high-level VSCF/VCI calculations. Journal of Chemical Physics, 2020, 153, 124506.	3.0	20
250	Reaction dynamics for O(3P)+H ₂ , D ₂ , and HD. VI. Comparison of TST and reduced dimensionality quantum and quasiclassical isotope effects with experiment. Journal of Chemical Physics, 1987, 86, 1976-1981.	3.0	19
251	Quantum scattering calculations for vibrational and rotational excitation of CO by hot hydrogen atoms. Journal of Chemical Physics, 1995, 102, 8800-8806.	3.0	19
252	Collisional quenching of OD ⁺ by H ₂ : Experimental and theoretical studies of the state-resolved OD ⁺ product distribution and branching fraction. Journal of Chemical Physics, 2010, 133, 164307.	3.0	19

#	ARTICLE	IF	CITATIONS
253	The Dynamics of Allyl Radical Dissociation. Journal of Physical Chemistry A, 2011, 115, 6797-6804.	2.5	19
254	Experiment and Theory Elucidate the Multichannel Predissociation Dynamics of the HCl Trimer: Breaking Up Is Hard To Do. Journal of Physical Chemistry A, 2014, 118, 8402-8410.	2.5	19
255	Calculations of Mode-Specific Tunneling of Double-Hydrogen Transfer in Porphycene Agree with and Illuminate Experiment. Journal of Physical Chemistry Letters, 2014, 5, 2723-2727.	4.6	19
256	Quasiclassical trajectory studies of rigid rotor-rigid surface scattering. II. Corrugated surface. Journal of Chemical Physics, 1984, 80, 2183-2190.	3.0	18
257	A truncation/recoupling method for eigenvalues and eigenvectors ideal for parallel computation. Theoretica Chimica Acta, 1991, 79, 215-224.	0.8	18
258	Isolated resonance decomposition of a multichannel S matrix: A test from the scattering of H+CO=HCO. Journal of Chemical Physics, 1992, 96, 2812-2818.	3.0	18
259	Complex L2 calculation of the variation of resonance widths of HOCl with total angular momentum. Journal of Chemical Physics, 1999, 111, 4933-4941.	3.0	18
260	All-Atom Calculation of the Normal Modes of Bacteriorhodopsin Using a Sliding Block Iterative Diagonalization Method. Journal of Chemical Theory and Computation, 2006, 2, 166-174.	5.3	18
261	Communications: Classical trajectory study of the postquenching dynamics of OH A ²⁺ by H ₂ initiated at conical intersections. Journal of Chemical Physics, 2010, 132, 091102.	3.0	18
262	Ab Initio Deconstruction of the Vibrational Relaxation Pathways of Dilute HOD in Ice Ih. Journal of the American Chemical Society, 2014, 136, 5888-5891.	13.7	18
263	Visible/Infrared Dissociation of NO ₃ : Roaming in the Dark or Roaming on the Ground?. Journal of Physical Chemistry A, 2015, 119, 7163-7168.	2.5	18
264	Quasiclassical trajectory calculations of He-LiF (001) diffraction scattering. Journal of Chemical Physics, 1975, 63, 5231-5234.	3.0	17
265	Inclusion and assessment of Renner-Teller coupling in transition state theory for \hat{I} states: Application to O(3P)+H ₂ . Journal of Chemical Physics, 1985, 82, 1866-1872.	3.0	17
266	Quantum scattering calculations of energy transfer and isomerization of HCN/HNC in collisions with Ar. Journal of Chemical Physics, 2000, 112, 4496-4505.	3.0	17
267	Roaming Dynamics in Formaldehyde-d ₂ Dissociation. Journal of Physical Chemistry A, 2009, 113, 15315-15319.	2.5	17
268	Quasiclassical trajectory study of fast H-atom collisions with acetylene. Journal of Chemical Physics, 2012, 136, 214313.	3.0	17
269	Trajectory and Model Studies of Collisions of Highly Excited Methane with Water Using an ab Initio Potential. Journal of Physical Chemistry A, 2015, 119, 12304-12317.	2.5	17
270	Vibrational second-order perturbation theory (VPT2) using local monomer normal modes. Molecular Physics, 2015, 113, 3964-3971.	1.7	17

#	ARTICLE	IF	CITATIONS
271	Quantum and classical IR spectra of (HCOOH) ₂ , (DCOOH) ₂ and (DCOOD) ₂ using <i>ab initio</i> potential energy and dipole moment surfaces. Faraday Discussions, 2018, 212, 33-49.	3.2	17
272	Coupling of Low- and High-Frequency Vibrational Modes: Broadening in the Infrared Spectrum of F ⁺ (H ₂ O) ₂ . Journal of Physical Chemistry Letters, 2013, 4, 2964-2969.	4.6	16
273	Five <i>ab initio</i> potential energy and dipole moment surfaces for hydrated NaCl and NaF. I. Two-body interactions. Journal of Chemical Physics, 2016, 144, 114311.	3.0	16
274	Ab Initio, Embedded Local-Monomer Calculations of Methane Vibrational Energies in Clathrate Hydrates. Journal of Physical Chemistry C, 2016, 120, 3167-3175.	3.1	16
275	Disentangling the Complex Vibrational Mechanics of the Protonated Water Trimer by Rational Control of Its Hydrogen Bonds. Journal of Physical Chemistry A, 2019, 123, 7965-7972.	2.5	16
276	Observation of the Low-Frequency Spectrum of the Water Trimer as a Sensitive Test of the Water-Trimer Potential and the Dipole-Moment Surface. Angewandte Chemie - International Edition, 2020, 59, 11399-11407.	13.8	16
277	Collision induced isomerization of a semirigid bender hydrogen cyanide. Journal of Chemical Physics, 1994, 101, 8564-8571.	3.0	15
278	Resonances in the cumulative reaction probability for a model electronically nonadiabatic reaction. Journal of Chemical Physics, 1996, 104, 7545-7553.	3.0	15
279	Beyond Born-Oppenheimer. Science, 2008, 319, 40-41.	12.6	15
280	Two Pathways for Dissociation of Highly Energized <i>syn</i> -CH ₃ CHOO to OH Plus Vinyloxy. Journal of Physical Chemistry Letters, 2016, 7, 3359-3364.	4.6	15
281	A reduced dimensionality quasiclassical and quantum study of the proton transfer reaction H ₃ O ⁺ +H ₂ O ⁺ →H ₂ O+H ₃ O ⁺ . Journal of Chemical Physics, 2004, 120, 7018-7023.	3.0	14
282	Enhancement of tunneling due to resonances in pre-barrier wells in chemical reactions. Chemical Physics, 2005, 308, 255-257.	1.9	14
283	Do H ₅ ⁺ and Its Isotopologues Have Rotational Spectra?. Journal of Physical Chemistry Letters, 2011, 2, 1405-1407.	4.6	14
284	MULTIMODE calculations of the infrared spectra of H ₇ ⁺ and D ₇ ⁺ using <i>ab initio</i> potential energy and dipole moment surfaces. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	14
285	Complex coordinate, self-consistent field calculations of vibrational resonance energies. Journal of Chemical Physics, 1982, 76, 5370-5374.	3.0	13
286	Quantum calculations of inelastic and dissociative scattering of HCO by Ar. Journal of Chemical Physics, 1998, 109, 1734-1742.	3.0	13
287	Wave vector modification of the infinite order sudden approximation. Journal of Chemical Physics, 1980, 73, 3699-3708.	3.0	12
288	Model studies of atom and molecule diffusion on surfaces. Journal of Chemical Physics, 1984, 80, 2191-2196.	3.0	12

#	ARTICLE	IF	CITATIONS
289	Self-consistent field investigation of vibrations of atomic adsorbates. Journal of Chemical Physics, 1987, 87, 2363-2369.	3.0	12
290	CONSTRUCTION OF A GLOBAL POTENTIAL ENERGY SURFACE FROM NOVEL AB INITIO MOLECULAR DYNAMICS FOR THE O(3P) + C3H3 REACTION. Journal of Theoretical and Computational Chemistry, 2005, 04, 163-173.	1.8	12
291	The MD17 datasets from the perspective of datasets for gas-phase "small"-molecule potentials. Journal of Chemical Physics, 2022, 156, .	3.0	12
292	An improved quasiclassical histogram method. Journal of Chemical Physics, 1977, 66, 1756-1757.	3.0	11
293	Reply to Comment by Thomas on "On rainbow scattering in inelastic molecular collisions". Journal of Chemical Physics, 1981, 74, 2664-2665.	3.0	11
294	Approximations based on the adiabatic treatment of rotation for resonances. Journal of Chemical Physics, 1997, 107, 9960-9965.	3.0	11
295	Two novel applications of Shepard-type interpolation for polyatomic systems: Reduced dimensionality HOCO and full dimensionality Ar-HCO. International Journal of Quantum Chemistry, 1997, 65, 965-973.	2.0	11
296	Theoretical study of the photodetachment spectroscopy of the IBr and IDBr anions. Journal of Chemical Physics, 2000, 113, 9479-9487.	3.0	11
297	Anharmonic rovibrational calculations of singlet cyclic C4 using a new <i>ab initio</i> potential and a quartic force field. Journal of Chemical Physics, 2013, 139, 224302.	3.0	11
298	Communication: MULTIMODE calculations of low-lying vibrational states of NO3 using an adiabatic potential energy surface. Journal of Chemical Physics, 2014, 141, 161104.	3.0	11
299	A combined crossed molecular beam and quasiclassical trajectory study of the Titan-relevant N(2D) + D2O reaction. Molecular Physics, 2015, 113, 2296-2301.	1.7	11
300	A Model For Energy Transfer in Collisions of Atoms with Highly Excited Molecules. Journal of Physical Chemistry A, 2015, 119, 4695-4710.	2.5	11
301	Velocity map imaging of OH radical products from IR activated (CH3)2COO Criegee intermediates. Journal of Chemical Physics, 2016, 145, 104307.	3.0	11
302	Assessing the Importance of the H ₂ O-H ₂ O Three-Body Interaction on the Vibrational Frequency Shift of H ₂ in the sII Clathrate Hydrate and Comparison with Experiment. Journal of Physical Chemistry A, 2019, 123, 329-335.	2.5	11
303	Classical trajectory-quantum forced oscillator study of gas-surface phonon scattering: He/Si(100)-(2Å-1). Journal of Chemical Physics, 1984, 81, 6277-6280.	3.0	10
304	Full-dimensional, <i>ab initio</i> potential energy surface for CH ₃ OH+CH ₃ OH. Molecular Physics, 2013, 111, 1964-1971.	1.7	10
305	Two-layer Gaussian-based MCTDH study of the S1 \rightarrow S0 vibronic absorption spectrum of formaldehyde using multiplicative neural network potentials. Journal of Chemical Physics, 2019, 151, 064121.	3.0	10
306	Wavepacket propagation for reactive scattering using real L2 eigenfunctions with damping. Physical Chemistry Chemical Physics, 2000, 2, 495-500.	2.8	9

#	ARTICLE	IF	CITATIONS
307	Accurate Potential Energy Surfaces and Beyond: Chemical Reactivity, Binding, Long-Range Interactions, and Spectroscopy. <i>Advances in Physical Chemistry</i> , 2012, 2012, 1-4.	2.0	9
308	Ultraviolet Photodissociation Dynamics of the 1-Propenyl Radical. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5248-5256.	2.5	9
309	Inelastic vibrational dynamics of CS in collision with H ₂ using a full-dimensional potential energy surface. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 28425-28434.	2.8	9
310	Quasiclassical simulations based on cluster models reveal vibration-facilitated roaming in the isomerization of CO adsorbed on NaCl. <i>Nature Chemistry</i> , 2021, 13, 249-254.	13.6	9
311	MULTIMODE Calculations of Vibrational Spectroscopy and 1d Interconformer Tunneling Dynamics in Glycine Using a Full-Dimensional Potential Energy Surface. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5346-5354.	2.5	9
312	Evidence for a rotational rainbow in inelastic hot atom experiments?. <i>Journal of Chemical Physics</i> , 1987, 86, 3046-3046.	3.0	8
313	Adiabatic Rotation, Centrifugal Sudden, and Exact Calculations of Rotationally Mediated Fermi Resonances in HOCl. <i>Journal of Physical Chemistry A</i> , 2001, 105, 2423-2426.	2.5	8
314	Calculating Feshbach resonances in HCO using an extension of Q _{im} -path theory. <i>International Journal of Quantum Chemistry</i> , 2017, 117, 139-145.	2.0	8
315	A new functional form for global potentials of floppy molecules. <i>Journal of Molecular Structure</i> , 1990, 224, 133-139.	3.6	7
316	Bend Excitation Is Predicted to Greatly Accelerate Isomerization of <i>trans</i> -Hydroxymethylene to Formaldehyde in the Deep Tunneling Region. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 124-128.	4.6	7
317	Spectral analyses of <i>trans</i> - and <i>cis</i> -DOCO transients via comb spectroscopy. <i>Molecular Physics</i> , 2018, 116, 3710-3717.	1.7	7
318	H atom Product Channels in the Ultraviolet Photodissociation of the 2-Propenyl Radical. <i>Journal of Physical Chemistry A</i> , 2019, 123, 9957-9965.	2.5	7
319	Theoretical studies of rotation induced Fermi resonances in HOCl. <i>Journal of Chemical Physics</i> , 1999, 111, 7290-7297.	3.0	6
320	State-to-State Reactive Scattering via Reall2Wave Packet Propagation for Reduced Dimensionality AB + CD Reactions. <i>Journal of Physical Chemistry A</i> , 2001, 105, 2502-2508.	2.5	6
321	The 'MULTIMODE' approach to ro-vibrational spectroscopy. <i>AIP Conference Proceedings</i> , 2012, , .	0.4	6
322	The Rovibrational Spectra of <i>trans</i> - and <i>cis</i> -HOCO, Calculated by MULTIMODE with ab Initio Potential Energy and Dipole Moment Surfaces. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1616-1626.	2.5	6
323	On the use of an adiabaticity criterion to reduce computation time in quasiclassical trajectory calculations. <i>Journal of Chemical Physics</i> , 1976, 64, 4229-4230.	3.0	5
324	Observation of the Low-Frequency Spectrum of the Water Dimer as a Sensitive Test of the Water Dimer Potential and Dipole Moment Surfaces. <i>Angewandte Chemie</i> , 2019, 131, 13253-13260.	2.0	5

#	ARTICLE	IF	CITATIONS
325	Diffusion Monte Carlo with fictitious masses finds holes in potential energy surfaces. Molecular Physics, 0, , .	1.7	5
326	Electronic relaxation and dissociation dynamics in formaldehyde: pump wavelength dependence. Physical Chemistry Chemical Physics, 2022, 24, 1779-1786.	2.8	5
327	Rotational distributions from resonances in H + H ₂ . International Journal of Quantum Chemistry, 1986, 30, 681-687.	2.0	4
328	A reduced dimensionality quantum calculation of the reaction of H ₂ with diamond (111) surface. Journal of Chemical Physics, 2000, 113, 779-788.	3.0	4
329	Experimental and Theoretical Studies of Roaming Dynamics in the Unimolecular Dissociation of CH ₃ NO ₂ to CH ₃ O+NO. Zeitschrift Fur Physikalische Chemie, 2013, , 130708000310008.	2.8	4
330	Does Infrared Multiphoton Dissociation of Vinyl Chloride Yield Cold Vinylidene?. Journal of Physical Chemistry Letters, 2015, 6, 2457-2462.	4.6	4
331	Classical energy transfer in forced oscillator models of inelastic scattering. Journal of Chemical Physics, 1987, 87, 6618-6622.	3.0	3
332	Predissociation dynamics of the HClâ€“(H ₂ O) ₃ tetramer: An experimental and theoretical investigation. Journal of Chemical Physics, 2018, 148, 204303.	3.0	3
333	Teaching vibrational spectra to assign themselves. Faraday Discussions, 2018, 212, 65-82.	3.2	3
334	Diffusion Monte Carlo Calculations of Zeroâ€“Point Energies of Methanol and Deuterated Methanol. Journal of Computational Chemistry, 2019, 40, 328-332.	3.3	3
335	New numerical approaches to the solution of the N-well SchrÃ¶dinger equation. International Journal of Quantum Chemistry, 1989, 35, 297-303.	2.0	2
336	Laplace transformation of the SchrÃ¶dinger equation: Application to scattering. Journal of Chemical Physics, 1978, 68, 2825.	3.0	1
337	Approximate Quantum Approaches to the Calculation of Resonances in Reactive and Nonreactive Scattering. ACS Symposium Series, 1984, , 43-62.	0.5	1
338	Model calculations of electronic excitation of Li adsorbed on LiF(001). Journal of Chemical Physics, 1991, 94, 801-805.	3.0	1
339	Ab initio Calculations of the Interaction Potentials of Ar-HCN and Ar-HCO. ACS Symposium Series, 1997, , 150-172.	0.5	1
340	Gas Phase Vibrational Spectroscopy of Strong Hydrogen Bonds. , 0, , 53-78.		1
341	Sudden approximation theory of vibrational excitation. International Journal of Quantum Chemistry, 2009, 16, 487-500.	2.0	1
342	Diatom-diatom reactive scattering in hypercylindrical coordinates. International Journal of Quantum Chemistry, 1989, 36, 115-126.	2.0	1

#	ARTICLE	IF	CITATIONS
343	MULTIMODE, The <i>n</i> -Mode Representation of the Potential and Illustrations to IR Spectra of Glycine and Two Protonated Water Clusters. , 2022, , 296-339.		1
344	HN2 and DN2 Resonance Spectra. ACS Symposium Series, 1992, , 37-47.	0.5	0
345	The Challenge of High-Resolution Dynamics: Rotationally Mediated Unimolecular Dissociation of HOCl. ACS Symposium Series, 2002, , 346-360.	0.5	0
346	Keiji Morokuma. Journal of Physical Chemistry A, 2018, 122, 880-881.	2.5	0
347	Frontispiz: Observation of the Low-Frequency Spectrum of the Water Trimer as a Sensitive Test of the Water-Trimer Potential and the Dipole-Moment Surface. Angewandte Chemie, 2020, 132, .	2.0	0
348	Observation of the Low-Frequency Spectrum of the Water Trimer as a Sensitive Test of the Water-Trimer Potential and the Dipole-Moment Surface. Angewandte Chemie, 2020, 132, 11496-11504.	2.0	0
349	Frontispiece: Observation of the Low-Frequency Spectrum of the Water Trimer as a Sensitive Test of the Water-Trimer Potential and the Dipole-Moment Surface. Angewandte Chemie - International Edition, 2020, 59, .	13.8	0
350	On the measurement of statistical dynamics using the method of Coulomb explosion imaging. AIP Conference Proceedings, 2021, , .	0.4	0
351	Reaction Pathways: <i>Intramolecular Motion and Chemical Reaction</i> . I. M. Mills, M. S. Child, and R. A. Marcus, Eds. Royal Society, London, 1990. viii, 198 pp., illus. £40. From a meeting, London, Feb. 1990. Reprinted from the <i>Philosophical Transactions of the Royal Society of London</i> , series A, vol. 332, no. 1625 (1990). Science, 1991, 252, 589-589.	12.6	0
352	Capturing Roaming Fragments in Real Time: A Molecular Road Movie. , 2020, , .		0