Yimin Wang

List of Publications by Year
in descending order

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		236833	254106
43	2,164	25	43
papers	citations	h-index	g-index

43	43	43	1378
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	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
3	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
4	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
5	Full-dimensional, ab initio potential energy and dipole moment surfaces for water. Journal of Chemical Physics, 2009, 131, 054511.	1.2	133
6	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
7	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
8	Towards an ab initio flexible potential for water, and post-harmonic quantum vibrational analysis of water clusters. Chemical Physics Letters, 2010, 491, 1-10.	1.2	96
9	<scp>MULTIMODE</scp> quantum calculations of intramolecular vibrational energies of the water dimer and trimer using ab initio-based potential energy surfaces. Journal of Chemical Physics, 2008, 128, 071101.	1.2	59
10	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
11	Shared-Proton Mode Lights up the Infrared Spectrum of Fluxional Cations H₅⁺ and D₅⁺. Journal of Physical Chemistry Letters, 2010, 1, 758-762.	2.1	52
12	Quasi-Classical Trajectory Study of the HO + CO â† H + CO₂ Reaction on a New ab Initio Based Potential Energy Surface. Journal of Physical Chemistry A, 2012, 116, 5057-5067.	1.1	51
13	Energetics and Predissociation Dynamics of Small Water, HCl, and Mixed HClâ€“Water Clusters. Chemical Reviews, 2016, 116, 4913-4936.	23.0	49
14	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
15	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
16	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
17	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
18	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

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19	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
20	One-dimensional tunneling calculations in the imaginary-frequency, rectilinear saddle-point normal mode. Journal of Chemical Physics, 2008, 129, 121103.	1.2	40
21	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
22	Communication: Quasiclassical trajectory calculations of correlated product-state distributions for the dissociation of (H2O)2 and (D2O)2. Journal of Chemical Physics, 2011, 135, 151102.	1.2	33
23	Transferable ab Initio Dipole Moment for Water: Three Applications to Bulk Water. Journal of Physical Chemistry B, 2016, 120, 1735-1742.	1.2	31
24	Dipole Surface and Infrared Intensities for the cis- and trans-HOCO and DOCO Radicals. Journal of Physical Chemistry A, 2013, 117, 6932-6939.	1.1	30
25	Ab Initio Quantum Approaches to the IR Spectroscopy of Water and Hydrates. Journal of Physical Chemistry Letters, 2015, 6, 366-373.	2.1	27
26	Quantum Local Monomer IR Spectrum of Liquid D₂O at 300 K from 0 to 4000 cm^{â€“1} Is in Near-Quantitative Agreement with Experiment. Journal of Physical Chemistry B, 2016, 120, 2824-2828.	1.2	25
27	Quantum vibrational analysis and infrared spectra of microhydrated sodium ions using an ab initio potential. Journal of Chemical Physics, 2011, 134, 114311.	1.2	23
28	Reduced-Dimensional Quantum Approach to Tunneling Splittings Using Saddle-Point Normal Coordinates. Journal of Physical Chemistry A, 2009, 113, 7556-7562.	1.1	22
29	Communication: Rigorous calculation of dissociation energies (D) of the water trimer, (H2O)3 and (D2O)3. Journal of Chemical Physics, 2011, 135, 131101.	1.2	22
30	Variational Calculations of Vibrational Energies and IR Spectra of trans- and cis-HOCO Using New ab Initio Potential Energy and Dipole Moment Surfaces. Journal of Physical Chemistry A, 2013, 117, 9343-9352.	1.1	22
31	Vibrational Analysis of an Ice Ih Model from 0 to 4000 cm^{â€“1} Using the Ab Initio WHBB Potential Energy Surface. Journal of Physical Chemistry B, 2013, 117, 10046-10052.	1.2	20
32	Local-Monomer Calculations of the Intramolecular IR Spectra of the Cage and Prism Isomers of HOD(D₂O)₅ and HOD and D₂O Ice Ih. Journal of Physical Chemistry B, 2014, 118, 14124-14131.	1.2	20
33	Ab Initio Deconstruction of the Vibrational Relaxation Pathways of Dilute HOD in Ice Ih. Journal of the American Chemical Society, 2014, 136, 5888-5891.	6.6	18
34	Calculations of the IR spectra of bend fundamentals of (H₂O)_{n=3,4,5} using the WHBB_2 potential and dipole moment surfaces. Physical Chemistry Chemical Physics, 2016, 18, 24057-24062.	1.3	18
35	Mechanistic Studies of O₂-Based Sulfoxidations Catalyzed by NO_x/Br Systems. ACS Catalysis, 2011, 1, 1364-1370.	5.5	16
36	Five ab initio potential energy and dipole moment surfaces for hydrated NaCl and NaF. I. Two-body interactions. Journal of Chemical Physics, 2016, 144, 114311.	1.2	16

#	Article	IF	Citations
37	Full-dimensional (15-dimensional) ab initio analytical potential energy surface for the ${m H}_7^+$H7+ cluster. Journal of Chemical Physics, 2012, 136, 224302.	1.2	15
38	Do H₅⁺ and Its Isotopologues Have Rotational Spectra?. Journal of Physical Chemistry Letters, 2011, 2, 1405-1407.	2.1	14
39	Communication: Prediction of the rate constant of bimolecular hydrogen exchange in the water dimer using an ab initio potential energy surface. Journal of Chemical Physics, 2010, 133, 111103.	1.2	7
40	Bend Excitation Is Predicted to Greatly Accelerate Isomerization of trans-Hydroxymethylene to Formaldehyde in the Deep Tunneling Region. Journal of Physical Chemistry Letters, 2015, 6, 124-128.	2.1	7
41	Spectral analyses of trans- and cis-DOCO transients via comb spectroscopy. Molecular Physics, 2018, 116, 3710-3717.	0.8	7
42	Calculations and measurements of the deuterium tunneling frequency in the propiolic acid-formic acid dimer and description of a newly constructed Fourier transform microwave spectrometer. Journal of Chemical Physics, 2013, 139, 084316.	1.2	6
43	The Rovibrational Spectra of trans- and cis-HOCO, Calculated by MULTIMODE with ab Initio Potential Energy and Dipole Moment Surfaces. Journal of Physical Chemistry A, 2017, 121, 1616-1626.	1.1	6