Xiao-gang Wang

List of Publications by Year
in descending order

86	3,021	147801 31	168389 53
papers	citations	h-index	g-index

87	87	87	1144
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A contracted basis-Lanczos calculation of vibrational levels of methane: Solving the SchrÃ¶dinger equation in nine dimensions. Journal of Chemical Physics, 2003, 119, 101-117.	3.0	177
2	A Nested Molecule-Independent Neural Network Approach for High-Quality Potential Fitsâ€. Journal of Physical Chemistry A, 2006, 110, 5295-5304.	2.5	166
3	Vibrational energy levels of CH5+. Journal of Chemical Physics, 2008, 129, 234102.	3.0	140
4	New ideas for using contracted basis functions with a Lanczos eigensolver for computing vibrational spectra of molecules with four or more atoms. Journal of Chemical Physics, 2002, 117, 6923-6934.	3.0	129
5	Methane line parameters in the HITRAN2012 database. Journal of Quantitative Spectroscopy and Radiative Transfer, 2013, 130, 201-219.	2.3	121
6	Contracted basis Lanczos methods for computing numerically exact rovibrational levels of methane. Journal of Chemical Physics, 2004, 121, 2937-2954.	3.0	117
7	A nine-dimensional perturbative treatment of the vibrations of methane and its isotopomers. Journal of Chemical Physics, 1999, 111, 4510-4522.	3.0	99
8	A symmetry-adapted Lanczos method for calculating energy levels with different symmetries from a single set of iterations. Journal of Chemical Physics, 2001, 114, 1473-1477.	3.0	99
9	Nitrous oxide dimer: A new potential energy surface and rovibrational spectrum of the nonpolar isomer. Journal of Chemical Physics, 2010, 133, 134304.	3.0	94
10	A finite basis representation Lanczos calculation of the bend energy levels of methane. Journal of Chemical Physics, 2003, 118, 6946-6956.	3.0	85
11	Six-dimensional variational calculation of the bending energy levels of HF trimer and DF trimer. Journal of Chemical Physics, 2001, 115, 9781-9796.	3.0	82
12	Computing rovibrational levels of methane with curvilinear internal vibrational coordinates and an Eckart frame. Journal of Chemical Physics, 2013, 138, 104106.	3.0	73
13	Quantum states of a sextic potential: hidden symmetry and quantum monodromy. Journal of Physics A, 2000, 33, 5653-5661.	1.6	71
14	Theoretical and experimental studies of the infrared rovibrational spectrum of He2â€“N2O. Journal of Chemical Physics, 2005, 123, 034301.	3.0	71
15	Anharmonic force field and vibrational frequencies of tetrafluoromethane (CF4) and tetrafluorosilane (SiF4). Journal of Chemical Physics, 2000, 112, 1353-1366.	3.0	64
16	Explicitly correlated MRCI-F12 potential energy surfaces for methane fit with several permutation invariant schemes and full-dimensional vibrational calculations. Molecular Physics, 2015, 113, 1823-1833.	1.7	63
17	The Utility of Constraining Basis Function Indices When Using the Lanczos Algorithm to Calculate Vibrational Energy Levelsâ€. Journal of Physical Chemistry A, 2001, 105, 2575-2581.	2.5	61
18	CO Dimer: New Potential Energy Surface and Rovibrational Calculations. Journal of Physical Chemistry A, 2013, 117, 7612-7630.	2.5	61

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19	Theoretical study of the rovibrational spectrum of H2Oâ€“H2. Journal of Chemical Physics, 2011, 134, 044313.	3.0	55
20	Computational study of the rovibrational spectrum of (OCS)2. Journal of Chemical Physics, 2012, 136, 134306.	3.0	55
21	Using experimental data and a contracted basis Lanczos method to determine an accurate methane potential energy surface from a least squares optimization. Journal of Chemical Physics, 2014, 141, 154106.	3.0	52
22	Using monomer vibrational wavefunctions to compute numerically exact (12D) rovibrational levels of water dimer. Journal of Chemical Physics, 2018, 148, 074108.	3.0	51
23	Analysis of the rovibrational spectrum of 13CH4 in the Octad range. Journal of Molecular Spectroscopy, 2013, 291, 33-47.	1.2	48
24	A simple method for deriving kinetic energy operators. Journal of Chemical Physics, 2000, 113, 7097-7101.	3.0	46
25	Vibrational spectra of halide-water dimers: Insights on ion hydration from full-dimensional quantum calculations on many-body potential energy surfaces. Journal of Chemical Physics, 2018, 148, 102321.	3.0	40
26	Calculated vibrational states of ozone up to dissociation. Journal of Chemical Physics, 2016, 144, 074302.	3.0	39
27	The vibrationâ€“rotationâ€“tunneling spectrum of the polar and T-shaped-N-in isomers of (NNO)2. Journal of Molecular Spectroscopy, 2011, 268, 53-65.	1.2	38
28	A perturbative calculation of the rovibrational energy levels of methane. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 863-872.	3.9	33
29	Improving the calculation of rovibrational spectra of five-atom molecules with three identical atoms by using a C3ì…(G6) symmetry-adapted grid: Applied to CH3D and CHD3. Journal of Chemical Physics, 2005, 123, 154303.	3.0	33
30	Calculated rotation-bending energy levels of CH5+ and a comparison with experiment. Journal of Chemical Physics, 2016, 144, 204304.	3.0	33
31	Computing roâ€vibrational spectra of van der Waals molecules. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 952-963.	14.6	32
32	Computational study of the rovibrational spectrum of CO2â€“CS2. Journal of Chemical Physics, 2014, 140, 114303.	3.0	30
33	A discrete variable representation method for studying the rovibrational quantum dynamics of molecules with more than three atoms. Journal of Chemical Physics, 2009, 130, 094101.	3.0	29
34	Using monomer vibrational wavefunctions as contracted basis functions to compute rovibrational levels of an H2O-atom complex in full dimensionality. Journal of Chemical Physics, 2017, 146, 104105.	3.0	28
35	Computational study of the rovibrational spectrum of (CO2)2. Journal of Molecular Spectroscopy, 2016, 330, 179-187.	1.2	27
36	The (5000) Local Mode Vibrational State of Germane: A High-Resolution Spectroscopic Study. Journal of Molecular Spectroscopy, 1997, 184, 12-21.	1.2	26

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37	A nine-dimensional high order perturbative study of the vibration of silane and its isotopomers. Journal of Chemical Physics, 2000, 113, 5384.	3.0	26
38	A multimode-like scheme for selecting the centers of Gaussian basis functions when computing vibrational spectra. Chemical Physics, 2018, 509, 139-144.	1.9	25
39	Rovibrational levels and wavefunctions of Clâ^'H2O. Journal of Chemical Physics, 2014, 140, 204306.	3.0	24
40	Deficiencies of the bend symmetry coordinates used for methane. Journal of Chemical Physics, 2003, 118, 6260-6263.	3.0	23
41	Using C3v symmetry with polyspherical coordinates for methane. Journal of Chemical Physics, 2003, 119, 94-100.	3.0	23
42	Computational study of the rovibrational spectra of CO2â€"C2H2 and CO2â€"C2D2. Journal of Molecular Spectroscopy, 2016, 330, 170-178.	1.2	23
43	Theoretical and Experimental Study of the Rovibrational Spectrum of He₂â^'CO. Journal of Physical Chemistry A, 2009, 113, 13331-13341.	2.5	22
44	High-Resolution Spectroscopic Study of the (310) Local Mode Combination Band System of AsH3. Journal of Molecular Spectroscopy, 1998, 187, 89-96.	1.2	21
45	USING LEBEDEV GRIDS, SINE SPHERICAL HARMONICS, AND MONOMER CONTRACTED BASIS FUNCTIONS TO CALCULATE BENDING ENERGY LEVELS OF HF TRIMER. Journal of Theoretical and Computational Chemistry, 2003, 02, 599-608.	1.8	20
46	Computational study of the ro-vibrational spectrum of COâ€"CO2. Journal of Chemical Physics, 2019, 151, 084307.	3.0	19
47	Theoretical and experimental study of infrared spectra of He₂-CO₂This article is part of a Special Issue on Spectroscopy at the University of New Brunswick in honour of Colan Linton and Ron Lees.. Canadian Journal of Physics, 2009, 87, 417-423.	1.1	18
48	Exact vibration-rotation kinetic energy operators in two sets of valence coordinates for centrally connected penta-atomic molecules. Molecular Physics, 2000, 98, 317-326.	1.7	17
49	Vibrational Levels of Ar4:Â New Odd-Parity Bosonic Statesâ€. Journal of Physical Chemistry A, 2007, 111, 10220-10225.	2.5	17
50	The vibrational overtones of SiH4 isotopomers: experimental wavenumbers, assignment, ab initio dipole moment surfaces and intensities. Physical Chemistry Chemical Physics, 2001, 3, 3506-3517.	2.8	14
51	K-independent vibrational bases for systems with large amplitude motion. Molecular Physics, 2012, 110, 825-835.	1.7	14
52	Ab initio study of the COâ€"N2 complex: a new highly accurate intermolecular potential energy surface and rovibrational spectrum. Physical Chemistry Chemical Physics, 2018, 20, 12624-12636.	2.8	14
53	High resolution spectroscopic study of CH₃D in the region 5900â€"6100 cm^{â^'1}. Molecular Physics, 1999, 97, 787-795.	1.7	13
54	Infrared spectrum and intermolecular potential energy surface of the COâ€"O₂ dimer. Physical Chemistry Chemical Physics, 2018, 20, 14431-14440.	2.8	13

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55	High resolution photoacoustic spectrum of AsH3 () bands. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1997, 53, 1705-1712.	3.9	12
56	Computational study of the rovibrational spectrum of CO2â€“N2. Physical Chemistry Chemical Physics, 2020, 22, 22674-22683.	2.8	12
57	Absorption Intensity of Stretching Overtone States of Silane and Germane. Journal of Molecular Spectroscopy, 1998, 192, 249-256.	1.2	11
58	The ab initio calculated dipole moment surface and overtone relative intensities of CH chromophore in CHCl3. Journal of Chemical Physics, 2000, 112, 7484-7489.	3.0	11
59	Using a nondirect product discrete variable representation for angular coordinates to compute vibrational levels of polyatomic molecules. Journal of Chemical Physics, 2008, 128, 194109.	3.0	11
60	Parallel methods for high-dimensional quantum dynamics. Computer Physics Communications, 2010, 181, 455-461.	7.5	11
61	Vibronic interaction in CO₃^{â˜} photo-detachment: Jahnâ€“Teller effects beyond structural distortion and general formalisms for vibronic Hamiltonians in trigonal symmetries. Physical Chemistry Chemical Physics, 2019, 21, 8679-8690.	2.8	11
62	Anharmonicity: a route to vibrational localization. Chemical Physics Letters, 1993, 212, 403-408.	2.6	10
63	The vibration-rotation-tunneling levels of N2â€“H2O and N2â€“D2O. Journal of Chemical Physics, 2015, 143, 024303.	3.0	10
64	Band strengths for Câ€“H stretching polyads of CHBr3 calculated by use of a two-dimensional electric dipole moment surface from density functional theory. Journal of Chemical Physics, 2001, 114, 8905-8912.	3.0	9
65	High-Resolution Rotational Analysis of thev= 6, 7, and 8 Geâ€“H Stretching Overtones of70GeHD3. Journal of Molecular Spectroscopy, 1996, 176, 9-16.	1.2	8
66	Calculating relative intensities for CH stretching polyads of CHI3 with ab initio dipole moment surface. Chemical Physics Letters, 2000, 332, 569-575.	2.6	8
67	The high resolution spectrum of AsH3 (400) local mode state: symmetry reduction and rotational re-quantization. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1998, 54, 1947-1960.	3.9	7
68	Theoretical study of the rovibrational spectrum of He₂â€“OCS. Canadian Journal of Chemistry, 2010, 88, 779-786.	1.1	7
69	Computing rovibrational levels of polyatomic molecules with polyspherical coordinates and a contracted basis built with a K-independent vibrational primitive basis. Molecular Physics, 2013, 111, 2320-2333.	1.7	7
70	Computing energy levels of CH4, CHD3, CH3D, and CH3F with a direct product basis and coordinates based on the methyl subsystem. Journal of Chemical Physics, 2018, 148, 074113.	3.0	7
71	Using nondirect product Wigner D basis functions and the symmetry-adapted Lanczos algorithm to compute the ro-vibrational spectrum of CH4â€“H2O. Journal of Chemical Physics, 2021, 154, 124112.	3.0	7
72	High resolution spectroscopic study of arsine in the region 6000â€“6500 cmâ˜1. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1998, 55, 109-119.	3.9	6

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73	A variational calculation of vibrational levels of vinyl radical. Journal of Chemical Physics, 2020, 152, 204311.	3.0	6
74	Computational study of the rovibrational spectrum of H<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e9065" altimg="si22.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:math>O-HF. Journal of Molecular Spectroscopy, 2022, 384, 111587.	1.2	6
75	Computational Study of the Rovibrational Spectra of CH₂D⁺ and CHD₂⁺. Journal of Physical Chemistry A, 2019, 123, 10281-10289.	2.5	5
76	Study of the Perpendicular Band Intensities of the CH Chromophore in CHCl3, CHBr3, and CHI3 with Three-Dimensional Dipole Moment Surface from Density Functional Calculations. Journal of Physical Chemistry A, 2001, 105, 8428-8433.	2.5	4
77	Using simply contracted basis functions with the Lanczos algorithm to calculate vibrational spectra. International Journal of Quantum Chemistry, 2004, 99, 556-566.	2.0	4
78	Calculating and assigning rovibrational energy levels of (15N2O)2, (15N14NO)2, 14N2Oâ€“15N2O and 15N14NOâ€“15N2O. Physical Chemistry Chemical Physics, 2013, 15, 19159.	2.8	3
79	Intermolecular vibrations of the CO2â€“CS2 complex: Experiment and theory agree, but understanding remains challenging. Journal of Molecular Spectroscopy, 2016, 330, 188-193.	1.2	3
80	Coriolis interaction in the local mode (n100;F2) combination states of GeH4. Molecular Physics, 2000, 98, 1409-1413.	1.7	2
81	Computing vibrational and ro-vibrational spectra of CH5+. AIP Conference Proceedings, 2015, , .	0.4	2
82	Using quadrature and an iterative eigensolver to compute fine-structure ro-vibrational levels of Van der Waals complexes: NH(Î£â^3)â€“He, O2(Î£gâ^3)â€“Ar, and O2(Î£gâ^3)â€“He. Journal of Chemical Physics, 2019, 151, 054101.	3.1	2
83	Computing vibrationâ€“rotation-tunnelling levels of HOD dimer. Physical Chemistry Chemical Physics, 2019, 21, 3527-3536.	2.8	2
84	Rovibrational spectra of molecules in small helium clusters. , 2012, , .		1
85	The He2-OCS complex: Comparison between theory and experiment. Chemical Physics Letters, 2018, 694, 35-39.	2.6	0
86	A Parallel Algorithm for Computing the Spectrum of CH $_5^+$. Lecture Notes in Computer Science, 2010, , 109-116.	1.3	0