Kiyoshi Yagi

List of Publications by Year
in descending order

63	2,451	159585 30	206112 48
papers	citations	h-index	g-index

66	66	66	1619
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Weight average approaches for predicting dynamical properties of biomolecules. Current Opinion in Structural Biology, 2022, 72, 88-94.	5.7	3
2	Computational Analysis on the Allostery of Tryptophan Synthase: Relationship between Î±/Î²-Ligand Binding and Distal Domain Closure. Journal of Physical Chemistry B, 2022, 126, 3300-3308.	2.6	5
3	Exploring the Minimum-Energy Pathways and Free-Energy Profiles of Enzymatic Reactions with QM/MM Calculations. Journal of Physical Chemistry B, 2021, 125, 4701-4713.	2.6	21
4	Anharmonic Vibrational Calculations Based on Group-Localized Coordinates: Applications to Internal Water Molecules in Bacteriorhodopsin. Journal of Chemical Theory and Computation, 2021, 17, 5007-5020.	5.3	8
5	Towards complete assignment of the infrared spectrum of the protonated water cluster H+(H2O)21. Nature Communications, 2021, 12, 6141.	12.8	35
6	Retinal Vibrations in Bacteriorhodopsin are Mechanically Harmonic but Electrically Anharmonic: Evidence From Overtone and Combination Bands. Frontiers in Molecular Biosciences, 2021, 8, 749261.	3.5	3
7	Amide A band is a fingerprint for water dynamics in reverse osmosis polyamide membranes. Journal of Membrane Science, 2020, 596, 117705.	8.2	15
8	Anharmonic Vibrational Analysis of Biomolecules and Solvated Molecules Using Hybrid QM/MM Computations. Journal of Chemical Theory and Computation, 2019, 15, 1924-1938.	5.3	30
9	Fundamental peak disappears upon binding of a noble gas: a case of the vibrational spectrum of PtCO in an argon matrix. Physical Chemistry Chemical Physics, 2018, 20, 3296-3302.	2.8	1
10	Weight-Averaged Anharmonic Vibrational Analysis of Hydration Structures of Polyamide 6. Journal of Physical Chemistry B, 2017, 121, 6050-6063.	2.6	11
11	Infrared Spectra of Protonated Water Clusters, H⁺(H₂O)₄, in Eigen and Zundel Forms Studied by Vibrational Quasi-Degenerate Perturbation Theory. Journal of Physical Chemistry A, 2017, 121, 2386-2398.	2.5	28
12	Dynamics of nitric oxide controlled by protein complex in bacterial system. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 9888-9893.	7.1	35
13	Vibrational energy transport in acetylbenzonitrile described by an ab initio-based quantum tier model. Chemical Physics, 2017, 482, 86-92.	1.9	11
14	Detection of Sphingomyelin Clusters by Raman Spectroscopy. Biophysical Journal, 2016, 111, 999-1007.	0.5	35
15	Anharmonic Vibrational Analyses of Pentapeptide Conformations Explored with Enhanced Sampling Simulations. Journal of Physical Chemistry B, 2016, 120, 10199-10213.	2.6	11
16	Development of Molecular Vibrational Structure Theory with an Explicit Account of Anharmonicity. Molecular Science, 2016, 10, A0085.	0.2	4
17	A weight averaged approach for predicting amide vibrational bands of a sphingomyelin bilayer. Physical Chemistry Chemical Physics, 2015, 17, 29113-29123.	2.8	13
18	Optimized coordinates in vibrational coupled cluster calculations. Journal of Chemical Physics, 2014, 140, .	3.0	56

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19	Response to â€œComment on â€˜Fermi resonance in solid CO2 under pressureâ€™â€•[J. Chem. Phys. 140, 177101 (2014)]. Journal of Chemical Physics, 2014, 140, 177102.	3.0	7
20	Vibrational quasi-degenerate perturbation theory with optimized coordinates: Applications to ethylene and trans-1,3-butadiene. Journal of Chemical Physics, 2014, 140, 084113.	3.0	46
21	A simple state-average procedure determining optimal coordinates for anharmonic vibrational calculations. Chemical Physics Letters, 2014, 610-611, 288-297.	2.6	29
22	Stacked base-pair structures of adenine nucleosides stabilized by the formation of hydrogen-bonding network involving the two sugar groups. Chemical Physics, 2013, 419, 84-89.	1.9	27
23	Gas-phase spectroscopy and anharmonic vibrational analysis of the 3-residue peptide Z-Pro-Leu-Gly-NH2 by the laser desorption supersonic jet technique. Chemical Physics, 2013, 419, 145-152.	1.9	13
24	Fermi resonance in solid CO2 under pressure. Journal of Chemical Physics, 2013, 138, 074501.	3.0	50
25	ATR-FTIR Analysis of the State of Water in a Sulfonated Block Poly(arylene ether sulfone ketone) Membrane and Proton Conductivity Measurement during the Hydration/Dehydration Cycle. Journal of Physical Chemistry C, 2013, 117, 3762-3771.	3.1	16
26	DISSOCIATIVE RECOMBINATION OF VIBRATIONALLY COLD CH⁺₃AND INTERSTELLAR IMPLICATIONS. Astrophysical Journal, 2012, 758, 55.	4.5	16
27	Hydrogen-Bond Network Transformation in Water-Cluster Anions Induced by the Complex Formation with Benzene. Journal of Physical Chemistry Letters, 2012, 3, 3571-3575.	4.6	2
28	Extensivity of Energy and Electronic and Vibrational Structure Methods for Crystals. Annual Review of Physical Chemistry, 2012, 63, 131-153.	10.8	21
29	Optimized coordinates for anharmonic vibrational structure theories. Journal of Chemical Physics, 2012, 137, 204118.	3.0	100
30	First-principles calculations on anharmonic vibrational frequencies of polyethylene and polyacetylene in the Î“ approximation. Journal of Chemical Physics, 2010, 133, 034110.	3.0	14
31	First-principles theories for anharmonic lattice vibrations. Journal of Chemical Physics, 2010, 133, 034109.	3.0	37
32	Theoretical Study on the Excess Electron Binding Mechanism in the [CH₃NO₂Â·(H₂O)_n]^{â^’} (n = 1â^’6) Anion Clusters. Journal of Physical Chemistry A, 2010, 114, 8939-8947.	2.5	12
33	Computational Interstellar Chemistry. Thirty Years of Astronomical Discovery With UKIRT, 2010, , 21-30.	0.3	0
34	Firstâ€Principles Quantum Calculations on the Infrared Spectrum and Vibrational Dynamics of the Guanineâ€Cytosine Base Pair. ChemPhysChem, 2009, 10, 1442-1444.	2.1	23
35	Coupledâ€cluster and manyâ€body perturbation study of energies, structures, and phonon dispersions of solid hydrogen fluoride. International Journal of Quantum Chemistry, 2009, 109, 1928-1939.	2.0	37
36	Quantum and classical vibrational relaxation dynamics of Nâ€methylacetamide on ab initio potential energy surfaces. International Journal of Quantum Chemistry, 2009, 109, 2047-2057.	2.0	22

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37	Infrared spectra of water molecule encapsulated inside fullerene studied by instantaneous vibrational analysis. International Journal of Quantum Chemistry, 2009, 109, 2080-2090.	2.0	27
38	On the coupling strength in potential energy surfaces for vibrational calculations. Chemical Physics Letters, 2009, 483, 138-142.	2.6	45
39	Anharmonic vibrational frequencies and vibrationally-averaged structures of key species in hydrocarbon combustion: HCO⁺, HCO, HNO, HOO, HOO^{â€“}, CH₃⁺, and CH₃. Molecular Physics, 2009, 107, 1283-1301.	1.7	38
40	On the Validity of the Bornâ˜Oppenheimer Separation and the Accuracy of Diagonal Corrections in Anharmonic Molecular Vibrations. Journal of Physical Chemistry A, 2009, 113, 12461-12469.	2.5	6
41	Predictive electronic and vibrational many-body methods for molecules and macromolecules. Chemical Physics Letters, 2008, 464, 123-134.	2.6	37
42	Vibrational quasi-degenerate perturbation theory: applications to fermi resonance in CO2, H2CO, and C6H6. Physical Chemistry Chemical Physics, 2008, 10, 1781.	2.8	112
43	Water Cluster Anions Studied by the Long-Range Corrected Density Functional Theory. Journal of Physical Chemistry A, 2008, 112, 9845-9853.	2.5	36
44	Anharmonic vibrational frequencies and vibrationally averaged structures and nuclear magnetic resonance parameters of FHFâ˜. Journal of Chemical Physics, 2008, 128, 214305.	3.0	30
45	Efficient configuration selection scheme for vibrational second-order perturbation theory. Journal of Chemical Physics, 2007, 127, 034111.	3.0	55
46	Fermi resonance in CO2: A combined electronic coupled-cluster and vibrational configuration-interaction prediction. Journal of Chemical Physics, 2007, 126, 124303.	3.0	47
47	Anharmonic vibrational state calculations in the electronic excited states studied by time-dependent density functional theory. Chemical Physics Letters, 2007, 436, 30-35.	2.6	12
48	Quantum dynamics of N-methylacetamide studied by the vibrational configuration interaction method. Chemical Physics Letters, 2007, 443, 6-11.	2.6	40
49	Multiresolution potential energy surfaces for vibrational state calculations. Theoretical Chemistry Accounts, 2007, 118, 681-691.	1.4	103
50	Franck-Condon factors based on anharmonic vibrational wave functions of polyatomic molecules. Journal of Chemical Physics, 2006, 125, 014109.	3.0	38
51	Unidirectional Electronic Ring Current Driven by a Few Cycle Circularly Polarized Laser Pulse:â€‰Quantum Model Simulations for Mgâ˜Porphyrin. Journal of the American Chemical Society, 2006, 128, 7043-7049.	13.7	242
52	Highly accurate potential-energy and dipole moment surfaces for vibrational state calculations of methane. Journal of Chemical Physics, 2006, 124, 064311.	3.0	38
53	A vibrational analysis of the 7-azaindole-water complex: Anharmonicities using the quartic force field. International Journal of Quantum Chemistry, 2005, 104, 758-772.	2.0	21
54	Nonadiabatic chemical dynamics in an intense laser field: Electronic wave packet coupled with classical nuclear motions. Journal of Chemical Physics, 2005, 123, 224103.	3.0	38

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55	Simple and accurate method to evaluate tunneling splitting in polyatomic molecules. Journal of Chemical Physics, 2004, 120, 5036-5045.	3.0	62
56	Ab initiovibrational state calculations with a quartic force field: Applications to H2CO, C2H4, CH3OH, CH3CCH, and C6H6. Journal of Chemical Physics, 2004, 121, 1383-1389.	3.0	166
57	The effect of spinâ€“orbit coupling on fast neutral chemical reaction O(3P)+CH3â†'CH3O. Journal of Chemical Physics, 2004, 120, 10395-10403.	3.0	10
58	Effect of out-of-plane vibration on the hydrogen atom transfer reaction in malonaldehyde. Chemical Physics Letters, 2004, 397, 435-440.	2.6	29
59	Ab initio potential energy surface for vibrational state calculations of H2CO. Journal of Chemical Physics, 2003, 118, 1653-1660.	3.0	45
60	Tunneling splitting in polyatomic molecules: Application to malonaldehyde. Journal of Chemical Physics, 2003, 119, 10-13.	3.0	84
61	A new analytic form ofab initiopotential energy function: An application to H2O. Journal of Chemical Physics, 2002, 116, 3963-3966.	3.0	39
62	Generation of full-dimensional potential energy surface of intramolecular hydrogen atom transfer in malonaldehyde and tunneling dynamics. Journal of Chemical Physics, 2001, 115, 10647-10655.	3.0	100
63	Direct vibrational self-consistent field method: Applications to H2O and H2CO. Journal of Chemical Physics, 2000, 113, 1005-1017.	3.0	150