

Kiyoshi Yagi

List of Publications by Year in descending order

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63
papers

2,451
citations

159585

30
h-index

206112

48
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66
all docs

66
docs citations

66
times ranked

1619
citing authors

#	ARTICLE	IF	CITATIONS
1	Unidirectional Electronic Ring Current Driven by a Few Cycle Circularly Polarized Laser Pulse: Quantum Model Simulations for Mg ²⁺ Porphyrin. Journal of the American Chemical Society, 2006, 128, 7043-7049.	13.7	242
2	Ab initio vibrational state calculations with a quartic force field: Applications to H ₂ CO, C ₂ H ₄ , CH ₃ OH, CH ₃ CCH, and C ₆ H ₆ . Journal of Chemical Physics, 2004, 121, 1383-1389.	3.0	166
3	Direct vibrational self-consistent field method: Applications to H ₂ O and H ₂ CO. Journal of Chemical Physics, 2000, 113, 1005-1017.	3.0	150
4	Vibrational quasi-degenerate perturbation theory: applications to fermi resonance in CO ₂ , H ₂ CO, and C ₆ H ₆ . Physical Chemistry Chemical Physics, 2008, 10, 1781.	2.8	112
5	Multiresolution potential energy surfaces for vibrational state calculations. Theoretical Chemistry Accounts, 2007, 118, 681-691.	1.4	103
6	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
7	Optimized coordinates for anharmonic vibrational structure theories. Journal of Chemical Physics, 2012, 137, 204118.	3.0	100
8	Tunneling splitting in polyatomic molecules: Application to malonaldehyde. Journal of Chemical Physics, 2003, 119, 10-13.	3.0	84
9	Simple and accurate method to evaluate tunneling splitting in polyatomic molecules. Journal of Chemical Physics, 2004, 120, 5036-5045.	3.0	62
10	Optimized coordinates in vibrational coupled cluster calculations. Journal of Chemical Physics, 2014, 140, .	3.0	56
11	Efficient configuration selection scheme for vibrational second-order perturbation theory. Journal of Chemical Physics, 2007, 127, 034111.	3.0	55
12	Fermi resonance in solid CO ₂ under pressure. Journal of Chemical Physics, 2013, 138, 074501.	3.0	50
13	Fermi resonance in CO ₂ : A combined electronic coupled-cluster and vibrational configuration-interaction prediction. Journal of Chemical Physics, 2007, 126, 124303.	3.0	47
14	Vibrational quasi-degenerate perturbation theory with optimized coordinates: Applications to ethylene and <i>trans</i> -1,3-butadiene. Journal of Chemical Physics, 2014, 140, 084113.	3.0	46
15	Ab initio potential energy surface for vibrational state calculations of H ₂ CO. Journal of Chemical Physics, 2003, 118, 1653-1660.	3.0	45
16	On the coupling strength in potential energy surfaces for vibrational calculations. Chemical Physics Letters, 2009, 483, 138-142.	2.6	45
17	Quantum dynamics of N-methylacetamide studied by the vibrational configuration interaction method. Chemical Physics Letters, 2007, 443, 6-11.	2.6	40
18	A new analytic form of ab initio potential energy function: An application to H ₂ O. Journal of Chemical Physics, 2002, 116, 3963-3966.	3.0	39

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19	Nonadiabatic chemical dynamics in an intense laser field: Electronic wave packet coupled with classical nuclear motions. <i>Journal of Chemical Physics</i> , 2005, 123, 224103.	3.0	38
20	Franck-Condon factors based on anharmonic vibrational wave functions of polyatomic molecules. <i>Journal of Chemical Physics</i> , 2006, 125, 014109.	3.0	38
21	Highly accurate potential-energy and dipole moment surfaces for vibrational state calculations of methane. <i>Journal of Chemical Physics</i> , 2006, 124, 064311.	3.0	38
22	Anharmonic vibrational frequencies and vibrationally-averaged structures of key species in hydrocarbon combustion: HCO^+ , HCO , HNO , HOO , HOO^- , CH_3^+ , and CH_3 . <i>Molecular Physics</i> , 2009, 107, 1283-1301.	1.7	38
23	Predictive electronic and vibrational many-body methods for molecules and macromolecules. <i>Chemical Physics Letters</i> , 2008, 464, 123-134.	2.6	37
24	Coupled-cluster and many-body perturbation study of energies, structures, and phonon dispersions of solid hydrogen fluoride. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 1928-1939.	2.0	37
25	First-principles theories for anharmonic lattice vibrations. <i>Journal of Chemical Physics</i> , 2010, 133, 034109.	3.0	37
26	Water Cluster Anions Studied by the Long-Range Corrected Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2008, 112, 9845-9853.	2.5	36
27	Detection of Sphingomyelin Clusters by Raman Spectroscopy. <i>Biophysical Journal</i> , 2016, 111, 999-1007.	0.5	35
28	Dynamics of nitric oxide controlled by protein complex in bacterial system. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 9888-9893.	7.1	35
29	Towards complete assignment of the infrared spectrum of the protonated water cluster $\text{H}^+(\text{H}_2\text{O})_{21}$. <i>Nature Communications</i> , 2021, 12, 6141.	12.8	35
30	Anharmonic vibrational frequencies and vibrationally averaged structures and nuclear magnetic resonance parameters of FH_2^+ . <i>Journal of Chemical Physics</i> , 2008, 128, 214305.	3.0	30
31	Anharmonic Vibrational Analysis of Biomolecules and Solvated Molecules Using Hybrid QM/MM Computations. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1924-1938.	5.3	30
32	Effect of out-of-plane vibration on the hydrogen atom transfer reaction in malonaldehyde. <i>Chemical Physics Letters</i> , 2004, 397, 435-440.	2.6	29
33	A simple state-average procedure determining optimal coordinates for anharmonic vibrational calculations. <i>Chemical Physics Letters</i> , 2014, 610-611, 288-297.	2.6	29
34	Infrared Spectra of Protonated Water Clusters, $\text{H}^+(\text{H}_2\text{O})_4$, in Eigen and Zundel Forms Studied by Vibrational Quasi-Degenerate Perturbation Theory. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2386-2398.	2.5	28
35	Infrared spectra of water molecule encapsulated inside fullerene studied by instantaneous vibrational analysis. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 2080-2090.	2.0	27
36	Stacked base-pair structures of adenine nucleosides stabilized by the formation of hydrogen-bonding network involving the two sugar groups. <i>Chemical Physics</i> , 2013, 419, 84-89.	1.9	27

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37	First-Principles Quantum Calculations on the Infrared Spectrum and Vibrational Dynamics of the Guanine-Cytosine Base Pair. <i>ChemPhysChem</i> , 2009, 10, 1442-1444.	2.1	23
38	Quantum and classical vibrational relaxation dynamics of N-methylacetamide on ab initio potential energy surfaces. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 2047-2057.	2.0	22
39	A vibrational analysis of the 7-azaindole-water complex: Anharmonicities using the quartic force field. <i>International Journal of Quantum Chemistry</i> , 2005, 104, 758-772.	2.0	21
40	Extensivity of Energy and Electronic and Vibrational Structure Methods for Crystals. <i>Annual Review of Physical Chemistry</i> , 2012, 63, 131-153.	10.8	21
41	Exploring the Minimum-Energy Pathways and Free-Energy Profiles of Enzymatic Reactions with QM/MM Calculations. <i>Journal of Physical Chemistry B</i> , 2021, 125, 4701-4713.	2.6	21
42	DISSOCIATIVE RECOMBINATION OF VIBRATIONALLY COLD CH ⁺ ₃ AND INTERSTELLAR IMPLICATIONS. <i>Astrophysical Journal</i> , 2012, 758, 55.	4.5	16
43	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. <i>Journal of Physical Chemistry C</i> , 2013, 117, 3762-3771.	3.1	16
44	Amide A band is a fingerprint for water dynamics in reverse osmosis polyamide membranes. <i>Journal of Membrane Science</i> , 2020, 596, 117705.	8.2	15
45	First-principles calculations on anharmonic vibrational frequencies of polyethylene and polyacetylene in the \hat{I}^4 approximation. <i>Journal of Chemical Physics</i> , 2010, 133, 034110.	3.0	14
46	Gas-phase spectroscopy and anharmonic vibrational analysis of the 3-residue peptide Z-Pro-Leu-Gly-NH ₂ by the laser desorption supersonic jet technique. <i>Chemical Physics</i> , 2013, 419, 145-152.	1.9	13
47	A weight averaged approach for predicting amide vibrational bands of a sphingomyelin bilayer. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 29113-29123.	2.8	13
48	Anharmonic vibrational state calculations in the electronic excited states studied by time-dependent density functional theory. <i>Chemical Physics Letters</i> , 2007, 436, 30-35.	2.6	12
49	Theoretical Study on the Excess Electron Binding Mechanism in the [CH ₃ NO ₂ ·(H ₂ O) _n] ⁺ (<i>n</i> = 1-6) Anion Clusters. <i>Journal of Physical Chemistry A</i> , 2010, 114, 8939-8947.	2.5	12
50	Anharmonic Vibrational Analyses of Pentapeptide Conformations Explored with Enhanced Sampling Simulations. <i>Journal of Physical Chemistry B</i> , 2016, 120, 10199-10213.	2.6	11
51	Weight-Averaged Anharmonic Vibrational Analysis of Hydration Structures of Polyamide 6. <i>Journal of Physical Chemistry B</i> , 2017, 121, 6050-6063.	2.6	11
52	Vibrational energy transport in acetylbenzotrile described by an ab initio-based quantum tier model. <i>Chemical Physics</i> , 2017, 482, 86-92.	1.9	11
53	The effect of spin-orbit coupling on fast neutral chemical reaction O(3P)+CH ₃ ⁺ CH ₃ O. <i>Journal of Chemical Physics</i> , 2004, 120, 10395-10403.	3.0	10
54	Anharmonic Vibrational Calculations Based on Group-Localized Coordinates: Applications to Internal Water Molecules in Bacteriorhodopsin. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5007-5020.	5.3	8

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55	Response to "Comment on "Fermi resonance in solid CO ₂ under pressure" [J. Chem. Phys. 140, 177101 (2014)]. Journal of Chemical Physics, 2014, 140, 177102.	3.0	7
56	On the Validity of the Born-Oppenheimer Separation and the Accuracy of Diagonal Corrections in Anharmonic Molecular Vibrations. Journal of Physical Chemistry A, 2009, 113, 12461-12469.	2.5	6
57	Computational Analysis on the Allostery of Tryptophan Synthase: Relationship between $\hat{\mu}^2$ -Ligand Binding and Distal Domain Closure. Journal of Physical Chemistry B, 2022, 126, 3300-3308.	2.6	5
58	Development of Molecular Vibrational Structure Theory with an Explicit Account of Anharmonicity. Molecular Science, 2016, 10, A0085.	0.2	4
59	Weight average approaches for predicting dynamical properties of biomolecules. Current Opinion in Structural Biology, 2022, 72, 88-94.	5.7	3
60	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
61	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
62	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
63	Computational Interstellar Chemistry. Thirty Years of Astronomical Discovery With UKIRT, 2010, , 21-30.	0.3	0