Hua-Gen Yu

List of Publications by Year
in descending order

63	1,923	293460	286692
papers	citations	24 h-index	43 g-index

63	63	63	1243
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Active Thermochemical Tables: The Partition Function of Hydroxymethyl (CH2OH) Revisited. Journal of Physical Chemistry A, 2019, 123, 4212-4231.	1.1	13
2	Infrared vibrational spectra of CH3+ and its deuterated isotopologues. AIP Advances, 2019, 9, .	0.6	6
3	On the gas-phase formation of the HCO radical: accurate quantum study of the H+CO radiative association. Monthly Notices of the Royal Astronomical Society, 2018, 475, 2545-2552.	1.6	12
4	A rigorous full-dimensional quantum dynamics study of tunneling splitting of rovibrational states of vinyl radical C2H3. Journal of Chemical Physics, 2017, 146, 224307.	1.2	15
5	A coherent discrete variable representation method on a sphere. Journal of Chemical Physics, 2017, 147, 094101.	1.2	2
6	Rotational and angular distributions of NO products from NO-Rg (Rg = He, Ne, Ar) complex photodissociation. Journal of Chemical Physics, 2016, 144, 044309.	1.2	11
7	An exact variational method to calculate rovibrational spectra of polyatomic molecules with large amplitude motion. Journal of Chemical Physics, 2016, 145, 084109.	1.2	10
8	Full-Dimensional Quantum Calculations of Vibrational Levels of NH₄⁺ and Isotopomers on An Accurate Ab Initio Potential Energy Surface. Journal of Physical Chemistry A, 2016, 120, 2185-2193.	1.1	5
9	Vibrational energy levels of the simplest Criegee intermediate (CH2OO) from full-dimensional Lanczos, MCTDH, and MULTIMODE calculations. Journal of Chemical Physics, 2015, 143, 084311.	1.2	9
10	Doppler-Resolved Kinetics of Saturation Recovery. Journal of Physical Chemistry A, 2015, 119, 7439-7450.	1.1	5
11	Neural network iterative diagonalization method to solve eigenvalue problems in quantum mechanics. Physical Chemistry Chemical Physics, 2015, 17, 14071-14082.	1.3	8
12	Multi-layer Lanczos iteration approach to calculations of vibrational energies and dipole transition intensities for polyatomic molecules. Journal of Chemical Physics, 2015, 142, 044106.	1.2	8
13	Accurate quantum dynamics calculations of vibrational spectrum of dideuteromethane CH2D2. Journal of Chemical Physics, 2015, 142, 194307.	1.2	5
14	Origin of Anomalous Electronic Circular Dichroism Spectrum of RuPt₂(tppz)₂Cl₂(PF₆)₄ in Acetonitrile. Journal of Physical Chemistry A, 2014, 118, 5400-5406.	1.1	1
15	A complex guided spectral transform Lanczos method for studying quantum resonance states. Journal of Chemical Physics, 2014, 141, 244114.	1.2	2
16	Quantum approaches to polyatomic reaction dynamics. International Reviews in Physical Chemistry, 2013, 32, 39-95.	0.9	47
17	Convert graphene sheets to boron nitride and boron nitrideâ€“carbon sheets via a carbon-substitution reaction. Applied Physics Letters, 2011, 98, .	1.5	60
18	Synthesis and optical properties of GaN/ZnO solid solution nanocrystals. Applied Physics Letters, 2010, 96, .	1.5	52

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19	A general rigorous quantum dynamics algorithm to calculate vibrational energy levels of pentaatomic molecules. Journal of Molecular Spectroscopy, 2009, 256, 287-298.	0.4	20
20	Ab Initio and RRKM Study of the Reaction of ClO with HOCO Radicals. Journal of Physical Chemistry A, 2009, 113, 12932-12941.	1.1	14
21	Spherical Electron Cloud Hopping Molecular Dynamics Simulation on Dissociative Recombination of Protonated Water. Journal of Physical Chemistry A, 2009, 113, 6555-6561.	1.1	2
22	Theoretical Study of the Reaction of CH₃ with HOCO Radicals. Journal of Physical Chemistry A, 2009, 113, 3844-3849.	1.1	15
23	Energetics and kinetics of the reaction of HOCO with hydrogen atoms. Journal of Chemical Physics, 2008, 128, 244315.	1.2	21
24	Ab initioand direct dynamics study of the reaction of Cl atoms with HOCO. Journal of Chemical Physics, 2008, 129, 064301.	1.2	19
25	Energetics and molecular dynamics of the reaction of HOCO with HO2 radicals. Journal of Chemical Physics, 2008, 129, 214307.	1.2	20
26	A spherical electron cloud hopping model for studying product branching ratios of dissociative recombination. Journal of Chemical Physics, 2008, 128, 194106.	1.2	6
27	Quantum force molecular dynamics study of the reaction of O atoms with HOCO. Journal of Chemical Physics, 2007, 127, 094302.	1.2	20
28	Quantum Molecular Dynamics Study of the Reaction of O2with HOCOâ€. Journal of Physical Chemistry A, 2006, 110, 5312-5316.	1.1	23
29	A clue to the diffuse structure in ultraviolet spectra of the GeCl2 A-X transition. Journal of Chemical Physics, 2006, 125, 114316.	1.2	2
30	A rigorous full-dimensional quantum dynamics calculation of the vibrational energies of H3O2â˜†. Journal of Chemical Physics, 2006, 125, 204306.	1.2	26
31	Direct ab Initio Dynamics Study of the OH + HOCO Reaction. Journal of Physical Chemistry A, 2005, 109, 5230-5236.	1.1	40
32	Ab Initio and Direct Dynamics Studies of the Reaction of Singlet Methylene with Acetylene and the Lifetime of the Cyclopropene Complex. Journal of Physical Chemistry A, 2005, 109, 1890-1896.	1.1	27
33	A coherent discrete variable representation method for multidimensional systems in physics. Journal of Chemical Physics, 2005, 122, 164107.	1.2	20
34	Converged quantum dynamics calculations of vibrational energies of CH4 and CH3D using an ab initio potential. Journal of Chemical Physics, 2004, 121, 6334-6340.	1.2	52
35	Full-dimensional quantum calculations of vibrational spectra of six-atom molecules. I. Theory and numerical results. Journal of Chemical Physics, 2004, 120, 2270-2284.	1.2	45
36	MRCI Calculations of the Lowest Potential Energy Surface for CH3OH and Direct ab Initio Dynamics Simulations of the O(1D) + CH4Reactionâ€. Journal of Physical Chemistry A, 2004, 108, 8615-8623.	1.1	58

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37	Exploring the Multiple Reaction Pathways for the H + cyc-C3H6 Reaction. Journal of Physical Chemistry A, 2004, 108, 10844-10849.	1.1	11
38	THEORETICAL DETERMINATION OF ROVIBRATIONAL ENERGIES AND ANOMALOUS ISOTOPIC EFFECT OF WEAKLY BOUND CLUSTER HXeOH. Journal of Theoretical and Computational Chemistry, 2003, 02, 573-581.	1.8	7
39	Vibrational energy levels of methyl cation. Journal of Chemical Physics, 2002, 117, 666-669.	1.2	18
40	Quantum dynamics of the photoinitiated unimolecular dissociation of HOCO. Journal of Chemical Physics, 2002, 117, 11139-11145.	1.2	24
41	Two-layer Lanczos iteration approach to molecular spectroscopic calculation. Journal of Chemical Physics, 2002, 117, 8190-8196.	1.2	81
42	An exact variational method to calculate vibrational energies of five atom molecules beyond the normal mode approach. Journal of Chemical Physics, 2002, 117, 2030-2037.	1.2	71
43	A K-dependent adiabatic approximation to the Rennerâ€“Teller effect for triatomic molecules. Journal of Chemical Physics, 2002, 116, 1435-1442.	1.2	25
44	A General Variational Algorithm to Calculate Vibrational Energy Levels of Tetraatomic Molecules. Journal of Molecular Spectroscopy, 2002, 214, 11-20.	0.4	86
45	Accelerating the calculation of the rovibrational energies of tetraatomic molecules using a two-layer Lanczos algorithm. Chemical Physics Letters, 2002, 365, 189-196.	1.2	17
46	An Interpolated ab Initio Quantum Scattering Study of the Temperature Dependence of the CH3+ HBr â†' CH4+ Br Reactionâ€. Journal of Physical Chemistry A, 2001, 105, 2240-2245.	1.1	21
47	Iterative diagonalization of a large sparse matrix using spectral transformation and filter diagonalization. Journal of Computational Methods in Sciences and Engineering, 2001, 1, 229-250.	0.1	4
48	A five-dimensional quantum scattering model for the type AB+XCD3â‡ŒABX+CD3 reaction in hyperspherical coordinates: Application to OH+CH4â‡ŒH2O+CH3. Journal of Chemical Physics, 2001, 114, 2967-2976.	1.2	23
49	Experimental and theoretical studies of the near-infrared spectrum of bromomethylene. Journal of Chemical Physics, 2001, 115, 5433-5444.	1.2	39
50	Interpolatedab initioquantum scattering for the reaction of OH with HCl. Journal of Chemical Physics, 2000, 113, 8936-8944.	1.2	38
51	Quantum theory of bimolecular chemical reactions. Reports on Progress in Physics, 2000, 63, 1001-1059.	8.1	158
52	Direct ab initio quantum scattering for the H2+OHâ†'H+H2O reaction using MÃ¸llerâ€“Plesset fourth order perturbation theory. Journal of Chemical Physics, 2000, 112, 3935-3937.	1.2	13
53	Quantum dynamics of the O(3P)+CH4â†'OH+CH3 reaction: An application of the rotating bond umbrella model and spectral transform subspace iteration. Journal of Chemical Physics, 2000, 112, 238-247.	1.2	65
54	A spectral transform minimum residual filter diagonalization method for interior eigenvalues of physical systems. Journal of Chemical Physics, 1999, 110, 11133-11140.	1.2	25

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55	A four dimensional quantum scattering study of the Cl+CH4â‡ŒHCl+CH3 reaction via spectral transform iteration. Journal of Chemical Physics, 1999, 110, 7233-7244.	1.2	87
56	Four-dimensional quantum scattering calculations on the H+CH4â†'H2+CH3 reaction. Journal of Chemical Physics, 1999, 111, 3508-3516.	1.2	109
57	Reaction dynamics of chlorine atom with methane: Dual-level ab initio analytic potential energy surface and isotope effects. Journal of Chemical Physics, 1999, 111, 6693-6704.	1.2	57
58	Calculation of quantum resonance energies and lifetimes via quasi-minimum residual filter diagonalization. Chemical Physics Letters, 1998, 283, 69-76.	1.2	41
59	A spectral transform Krylov subspace iteration approach to quantum scattering. Chemical Physics Letters, 1998, 298, 27-35.	1.2	38
60	The simulation of outgoing-wave boundary conditions via a symmetrically damped, Hermitian Hamiltonian operator. Journal of Chemical Physics, 1997, 107, 9985-9993.	1.2	24
61	Restarted Krylov-space spectral filtering. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 861-869.	1.7	17
62	The calculation of vibrational eigenstates by MINRES filter diagonalization. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1997, 101, 400-406.	0.9	95
63	An efficient grid calculation of vibrational states for H3âˆ— with geometric phase in hyperspherical coordinates. Chemical Physics Letters, 1997, 281, 312-318.	1.2	28