Tucker Carrington

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4885225/publications.pdf

Version: 2024-02-01

232 papers	11,081 citations	24978 57 h-index	38300 95 g-index
245 all docs	245 docs citations	245 times ranked	3189 citing authors

#	Article	IF	Citations
1	Discrete-Variable Representations and their Utilization. Advances in Chemical Physics, 2007, , 263-310.	0.3	496
2	Variational quantum approaches for computing vibrational energies of polyatomic molecules. Molecular Physics, 2008, 106, 2145-2182.	0.8	402
3	A general discrete variable method to calculate vibrational energy levels of threeâ€•and fourâ€atom molecules. Journal of Chemical Physics, 1993, 99, 8519-8541.	1.2	359
4	The discrete variable representation of a triatomic Hamiltonian in bond lengthâ€“bond angle coordinates. Journal of Chemical Physics, 1992, 97, 3029-3037.	1.2	340
5	Reaction surface description of intramolecular hydrogen atom transfer in malonaldehyde. Journal of Chemical Physics, 1986, 84, 4364-4370.	1.2	265
6	Fermi resonances and local modes in water, hydrogen sulfide, and hydrogen selenide. Journal of Chemical Physics, 1988, 88, 4171-4185.	1.2	228
7	Angular Momentum Distribution and Emission Spectrum of OH (2Îź+) in the Photodissociation of H2O. Journal of Chemical Physics, 1964, 41, 2012-2018.	1.2	211
8	A random-sampling high dimensional model representation neural network for building potential energy surfaces. Journal of Chemical Physics, 2006, 125, 084109.	1.2	211
9	Efficient calculation of highly excited vibrational energy levels of floppy molecules: The band origins of H+3up to 35â€‰000 cmâ¯1. Journal of Chemical Physics, 1994, 100, 6175-6194.	1.2	196
10	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.	1.2	177
11	Neural networkâ€based approaches for building high dimensional and quantum dynamicsâ€friendly potential energy surfaces. International Journal of Quantum Chemistry, 2015, 115, 1012-1020.	1.0	170
12	Vinylidene: Potential energy surface and unimolecular reaction dynamics. Journal of Chemical Physics, 1984, 80, 4347-4354.	1.2	169
13	A Nested Molecule-Independent Neural Network Approach for High-Quality Potential Fitsâ€. Journal of Physical Chemistry A, 2006, 110, 5295-5304.	1.1	166
14	Neural Network Potential Energy Surfaces for Small Molecules and Reactions. Chemical Reviews, 2021, 121, 10187-10217.	23.0	163
15	Neural networks vs Gaussian process regression for representing potential energy surfaces: A comparative study of fit quality and vibrational spectrum accuracy. Journal of Chemical Physics, 2018, 148, 241702.	1.2	157
16	Using neural networks to represent potential surfaces as sums of products. Journal of Chemical Physics, 2006, 125, 194105.	1.2	156
17	Reaction surface Hamiltonian for the dynamics of reactions in polyatomic systems. Journal of Chemical Physics, 1984, 81, 3942-3950.	1.2	140
18	Vibrational energy levels of CH5+. Journal of Chemical Physics, 2008, 129, 234102.	1.2	140

#	Article	IF	Citations
19	The structure of Nb3O and Nb3O+ determined by pulsed field ionizationâ€“zero electron kinetic energy photoelectron spectroscopy and density functional theory. Journal of Chemical Physics, 1995, 103, 5335-5342.	1.2	135
20	Calculation of triatomic vibrational eigenstates: Product or contracted basis sets, Lanczos or conventional eigensolvers? What is the most efficient combination?. Journal of Chemical Physics, 1994, 101, 8494-8507.	1.2	133
21	A general framework for discrete variable representation basis sets. Journal of Chemical Physics, 2002, 116, 8691-8703.	1.2	129
22	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.	1.2	129
23	Methane line parameters in the HITRAN2012 database. Journal of Quantitative Spectroscopy and Radiative Transfer, 2013, 130, 201-219.	1.1	121
24	Contracted basis Lanczos methods for computing numerically exact rovibrational levels of methane. Journal of Chemical Physics, 2004, 121, 2937-2954.	1.2	117
25	Using a pruned basis, a non-product quadrature grid, and the exact Watson normal-coordinate kinetic energy operator to solve the vibrational SchrÃ¶dinger equation for C2H4. Journal of Chemical Physics, 2011, 135, 064101.	1.2	115
26	Calculation of vibrational fundamental and overtone band intensities of H2O. Journal of Chemical Physics, 1994, 100, 6228-6239.	1.2	112
27	Geometry of intersecting potential surfaces. Accounts of Chemical Research, 1974, 7, 20-25.	7.6	108
28	Using nonproduct quadrature grids to solve the vibrational SchrÃ¶dinger equation in 12D. Journal of Chemical Physics, 2011, 134, 054126.	1.2	108
29	Using neural networks, optimized coordinates, and high-dimensional model representations to obtain a vinyl bromide potential surface. Journal of Chemical Physics, 2008, 129, 224104.	1.2	100
30	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.	1.2	99
31	Nonproduct quadrature grids for solving the vibrational SchrÃ¶dinger equation. Journal of Chemical Physics, 2009, 131, 174103.	1.2	99
32	Nitrous oxide dimer: A new potential energy surface and rovibrational spectrum of the nonpolar isomer. Journal of Chemical Physics, 2010, 133, 134304.	1.2	94
33	Using redundant coordinates to represent potential energy surfaces with lower-dimensional functions. Journal of Chemical Physics, 2007, 127, 014103.	1.2	93
34	A new iterative method for calculating energy levels and wave functions. Journal of Chemical Physics, 2000, 112, 8765-8771.	1.2	88
35	A finite basis representation Lanczos calculation of the bend energy levels of methane. Journal of Chemical Physics, 2003, 118, 6946-6956.	1.2	85
36	Calculating vibrational energies and wave functions of vinylidene using a contracted basis with a locally reorthogonalized coupled two-term Lanczos eigensolver. Journal of Chemical Physics, 2006, 125, 094311.	1.2	85

#	Article	IF	Citations
37	Perspective: Computing (ro-)vibrational spectra of molecules with more than four atoms. Journal of Chemical Physics, 2017, 146, 120902.	1.2	83
38	Six-dimensional variational calculation of the bending energy levels of HF trimer and DF trimer. Journal of Chemical Physics, 2001, 115, 9781-9796.	1.2	82
39	Vibrational energy levels of formaldehyde calculated from an internal coordinate hamiltonian using the Lanczos algorithm. Chemical Physics Letters, 1993, 202, 464-470.	1.2	81
40	How to choose one-dimensional basis functions so that a very efficient multidimensional basis may be extracted from a direct product of the one-dimensional functions: Energy levels of coupled systems with as many as 16 coordinates. Journal of Chemical Physics, 2005, 122, 134101.	1.2	80
41	Accelerating the calculation of energy levels and wave functions using an efficient preconditioner with the inexact spectral transform method. Journal of Chemical Physics, 2001, 114, 9254-9264.	1.2	78
42	A preconditioned inexact spectral transform method for calculating resonance energies and widths, as applied to HCO. Journal of Chemical Physics, 2002, 116, 1215-1227.	1.2	74
43	Computing rovibrational levels of methane with curvilinear internal vibrational coordinates and an Eckart frame. Journal of Chemical Physics, 2013, 138, 104106.	1.2	73
44	Vibrational and geometric structures of Nb3C2 and Nb3C+2 from pulsed field ionizationâ€zero electron kinetic energy photoelectron spectra and density functional calculations. Journal of Chemical Physics, 1996, 105, 10663-10671.	1.2	71
45	Theoretical and experimental studies of the infrared rovibrational spectrum of He2â€“N2O. Journal of Chemical Physics, 2005, 123, 034301.	1.2	71
46	Calculating vibrational spectra with sum of product basis functions without storing full-dimensional vectors or matrices. Journal of Chemical Physics, 2014, 140, 174111.	1.2	70
47	Roadmap on Machine learning in electronic structure. Electronic Structure, 2022, 4, 023004.	1.0	69
48	Chemiluminescence during the course of a reactive encounter; F+Na2â†'FNaNaâ€¡*â†'NaF+Na*. Journal of Chemical Physics, 1980, 73, 5895-5897.	1.2	64
49	Discrete variable representations of complicated kinetic energy operators. Journal of Chemical Physics, 1994, 101, 1343-1360.	1.2	64
50	A comparison of filter diagonalisation methods with the Lanczos method for calculating vibrational energy levels. Chemical Physics Letters, 1999, 312, 311-318.	1.2	63
51	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.	0.8	63
52	Absolute rate constants for the reactions of CH with O and N atoms. Journal of Chemical Physics, 1981, 74, 3874-3881.	1.2	62
53	Solving the vibrational SchrÃ¶dinger equation using bases pruned to include strongly coupled functions and compatible quadratures. Journal of Chemical Physics, 2012, 137, 174108.	1.2	62
54	Absolute rate constants for the reactions of CH(X2II) with NO, N2O, NO2 and N2 at room temperature. Chemical Physics, 1982, 69, 61-70.	0.9	61

#	Article	IF	Citations
55	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.	1.1	61
56	CO Dimer: New Potential Energy Surface and Rovibrational Calculations. Journal of Physical Chemistry A, 2013, 117, 7612-7630.	1.1	61
57	An ab initio semirigid bender calculation of the rotation and transâ€tunneling spectra of (HF)2 and (DF)2. Journal of Chemical Physics, 1989, 91, 5154-5159.	1.2	59
58	Calculating rovibrational energy levels of a triatomic molecule with a simple Lanczos method. Journal of Chemical Physics, 1999, 110, 10269-10274.	1.2	57
59	Semiclassically optimized complex absorbing potentials of polynomial form. I. Pure imaginary case. Journal of Chemical Physics, 2003, 118, 17-28.	1.2	57
60	Theoretical study of the rovibrational spectrum of H2Oâ€“H2. Journal of Chemical Physics, 2011, 134, 044313.	1.2	55
61	Computational study of the rovibrational spectrum of (OCS)2. Journal of Chemical Physics, 2012, 136, 134306.	1.2	55
62	Predissociation and its inverse, using resonance absorption NO(Câ€‰2Î) â‡„ N+O. Journal of Chemical Physics, 1973, 58, 84-90.	1.2	54
63	Calculation of vibrational (J=0) excitation energies and band intensities of formaldehyde using the recursive residue generation method. Journal of Chemical Physics, 1996, 104, 7807-7820.	1.2	54
64	An exact Eckart-embedded kinetic energy operator in Radau coordinates for triatomic molecules. Chemical Physics Letters, 1998, 287, 289-300.	1.2	53
65	V3: Structure and vibrations from density functional theory, Franckâ€“Condon factors, and the pulsed-field ionization zero-electron-kinetic energy spectrum. Journal of Chemical Physics, 2001, 114, 4036-4044.	1.2	53
66	The reactions of C(21D2) with H2, D2 and HD: Product rotational energies, isotope effects and the CD/CH branching ratio. Chemical Physics, 1985, 97, 433-448.	0.9	52
67	An evaluation of methods designed to calculate energy levels in a selected range and application to a (oneâ€dimensional) Morse oscillator and (threeâ€dimensional) HCN/HNC. Journal of Chemical Physics, 1995, 103, 5600-5612.	1.2	52
68	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.	1.2	52
69	Using monomer vibrational wavefunctions to compute numerically exact (12D) rovibrational levels of water dimer. Journal of Chemical Physics, 2018, 148, 074108.	1.2	51
70	Fitting sparse multidimensional data with low-dimensional terms. Computer Physics Communications, 2009, 180, 2002-2012.	3.0	50
71	Explicit expressions for triatomic Eckart frames in Jacobi, Radau, and bond coordinates. Journal of Chemical Physics, 1997, 107, 2813-2818.	1.2	49
72	Using Nested Contractions and a Hierarchical Tensor Format To Compute Vibrational Spectra of Molecules with Seven Atoms. Journal of Physical Chemistry A, 2015, 119, 13074-13091.	1.1	49

#	Article	IF	Citations
73	Analysis of the rovibrational spectrum of 13CH4 in the Octad range. Journal of Molecular Spectroscopy, 2013, 291, 33-47.	0.4	48
74	The triatomic Eckart-frame kinetic energy operator in bond coordinates. Journal of Chemical Physics, 1997, 107, 9493-9501.	1.2	46
75	A simple method for deriving kinetic energy operators. Journal of Chemical Physics, 2000, 113, 7097-7101.	1.2	46
76	A multidimensional discrete variable representation basis obtained by simultaneous diagonalization. Journal of Chemical Physics, 2004, 121, 726-736.	1.2	46
77	Solving the Schroedinger equation using Smolyak interpolants. Journal of Chemical Physics, 2013, 139, 134114.	1.2	46
78	Investigation of fermi resonances in CHX3 molecules with an internal-coordinate hamiltonian. Journal of the Chemical Society, Faraday Transactions 2, 1988, 84, 1371.	1.1	45
79	Direct measurement of thermal rate constants for stateâ€toâ€state rotational energy transfer in collisions of CN(Xâ€‰2Î£+, v=2, N) with He. Journal of Chemical Physics, 1994, 100, 1190-1201.	1.2	44
80	Using preconditioned adaptive step size Runge-Kutta methods for solving the time-dependent SchrÃ¶dinger equation. Journal of Chemical Physics, 2004, 121, 11535-11541.	1.2	44
81	Photodissociation of ICN at 351, 337, and 308 nm. Rotational and vibrational energy disposal in CN(X2Î£+). Chemical Physics, 1983, 82, 443-457.	0.9	42
82	Photodissociation of BrCN and ICN in the a continuum: Vibrational and rotational distributions of CN(X 2Î£+). Chemical Physics, 1984, 89, 457-471.	0.9	41
83	Fermi resonance in CHX3: a hamiltonian in symmetrized curvilinear internal coordinates. Chemical Physics Letters, 1987, 140, 512-519.	1.2	40
84	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.	1.2	40
85	Calculated vibrational states of ozone up to dissociation. Journal of Chemical Physics, 2016, 144, 074302.	1.2	39
86	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.	0.4	38
87	Quenching and radiative lifetimes for NH(b1Î£+, Ï…â€² = 0). Chemical Physics Letters, 1975, 36, 238-241.	1.2	36
88	Using an expanding nondirect product harmonic basis with an iterative eigensolver to compute vibrational energy levels with as many as seven atoms. Journal of Chemical Physics, 2016, 145, 144104.	1.2	36
89	Semiclassically optimized complex absorbing potentials of polynomial form. II. Complex case. Journal of Chemical Physics, 2003, 119, 77-89.	1.2	35
90	Improving the calculation of rovibrational spectra of five-atom molecules with three identical atoms by using a C3Ï…(G6) symmetry-adapted grid: Applied to CH3D and CHD3. Journal of Chemical Physics, 2005, 123, 154303.	1.2	33

#	Article	IF	Citations
91	A multi-dimensional Smolyak collocation method in curvilinear coordinates for computing vibrational spectra. Journal of Chemical Physics, 2015, 143, 214108.	1.2	33
92	Calculated rotation-bending energy levels of CH5+ and a comparison with experiment. Journal of Chemical Physics, 2016, 144, 204304.	1.2	33
93	Computing roâ€vibrational spectra of van der Waals molecules. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 952-963.	6.2	32
94	Approximate First-Principles Anharmonic Calculations of Polyatomic Spectra Using MP2 and B3LYP Potentials: Comparisons with Experiment. Journal of Physical Chemistry A, 2014, 118, 6730-6739.	1.1	32
95	Using an internal coordinate Gaussian basis and a space-fixed Cartesian coordinate kinetic energy operator to compute a vibrational spectrum with rectangular collocation. Journal of Chemical Physics, 2016, 145, 224110.	1.2	32
96	Molecular beam chemiluminescence XI: kinetic and internal energy dependence of the NO + O3 â†' NO2*,â†' NO2â€¡ reaction. Chemical Physics, 1978, 27, 409-431.	0.9	31
97	Methods for calculating vibrational energy levels. Canadian Journal of Chemistry, 2004, 82, 900-914.	0.6	31
98	Using simultaneous diagonalization and trace minimization to make an efficient and simple multidimensional basis for solving the vibrational SchrÃ¶dinger equation. Journal of Chemical Physics, 2006, 124, 054102.	1.2	31
99	Computing vibrational energy levels by using mappings to fully exploit the structure of a pruned product basis. Journal of Chemical Physics, 2009, 130, 214110.	1.2	30
100	Computational study of the rovibrational spectrum of CO2â€“CS2. Journal of Chemical Physics, 2014, 140, 114303.	1.2	30
101	Computing the Anharmonic Vibrational Spectrum of UF₆ in 15 Dimensions with an Optimized Basis Set and Rectangular Collocation. Journal of Physical Chemistry A, 2015, 119, 9557-9567.	1.1	30
102	Adiabatic approach to the coupling between localâ€and normalâ€like modes. Journal of Chemical Physics, 1987, 86, 2207-2223.	1.2	29
103	Rotational energy transfer in collisions between CN (X, Î½ = 2) and argon. Comparison with results for helium. Chemical Physics Letters, 1995, 232, 547-553.	1.2	29
104	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.	1.2	29
105	On the advantages of a rectangular matrix collocation equation for computing vibrational spectra from small basis sets. Chemical Physics Letters, 2011, 511, 434-439.	1.2	29
106	Using a pruned, nondirect product basis in conjunction with the multi-configuration time-dependent Hartree (MCTDH) method. Journal of Chemical Physics, 2016, 145, 044110.	1.2	29
107	Calculation of reaction probabilities using wavepackets. Chemical Physics Letters, 1997, 267, 417-421.	1.2	28
108	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.	1.2	28

#	Article	IF	Citations
109	Using an iterative eigensolver and intertwined rank reduction to compute vibrational spectra of molecules with more than a dozen atoms: Uracil and naphthalene. Journal of Chemical Physics, 2018, 149, 064108.	1.2	28
110	Using a neural network based method to solve the vibrational SchrÃ¶dinger equation for H2O. Chemical Physics Letters, 2009, 474, 217-221.	1.2	27
111	Computational study of the rovibrational spectrum of (CO2)2. Journal of Molecular Spectroscopy, 2016, 330, 179-187.	0.4	27
112	Cross sections and energy disposal for cyanogen(X) produced in the hydrogen atom + hydrogen cyanide reaction at 53 and 58 kcal mol-1 collision energies. The Journal of Physical Chemistry, 1993, 97, 128-133.	2.9	26
113	Effect of rotation and vibration on nuclear magnetic resonance chemical shifts: Density functional theory calculations. Journal of Chemical Physics, 1999, 110, 7153-7159.	1.2	26
114	An intertwined method for making low-rank, sum-of-product basis functions that makes it possible to compute vibrational spectra of molecules with more than 10 atoms. Journal of Chemical Physics, 2017, 146, 204110.	1.2	26
115	Systematically expanding nondirect product bases within the pruned multi-configuration time-dependent Hartree (MCTDH) method: A comparison with multi-layer MCTDH. Journal of Chemical Physics, 2017, 146, 194105.	1.2	26
116	A multimode-like scheme for selecting the centers of Gaussian basis functions when computing vibrational spectra. Chemical Physics, 2018, 509, 139-144.	0.9	25
117	Anharmonic vibrations of the carboxyl group in acetic acid on TiO2: implications for adsorption mode assignment in dye-sensitized solar cells. Physical Chemistry Chemical Physics, 2013, 15, 10028.	1.3	24
118	Rovibrational levels and wavefunctions of Clâ¯H2O. Journal of Chemical Physics, 2014, 140, 204306.	1.2	24
119	Deficiencies of the bend symmetry coordinates used for methane. Journal of Chemical Physics, 2003, 118, 6260-6263.	1.2	23
120	Using C3v symmetry with polyspherical coordinates for methane. Journal of Chemical Physics, 2003, 119, 94-100.	1.2	23
121	Calculating anharmonic vibrational frequencies of molecules adsorbed on surfaces directly from ab initio energies with a molecule-independent method: H2O on Pt(111). Surface Science, 2011, 605, 616-622.	0.8	23
122	Using multi-dimensional Smolyak interpolation to make a sum-of-products potential. Journal of Chemical Physics, 2015, 143, 044106.	1.2	23
123	Using an iterative eigensolver to compute vibrational energies with phase-spaced localized basis functions. Journal of Chemical Physics, 2015, 143, 044104.	1.2	23
124	Computational study of the rovibrational spectra of CO2â€“C2H2 and CO2â€“C2D2. Journal of Molecular Spectroscopy, 2016, 330, 170-178.	0.4	23
125	Pruned bases that are compatible with iterative eigensolvers and general potentials: New results for CH3CN. Chemical Physics, 2017, 482, 3-8.	0.9	23
126	A new collocation-based multi-configuration time-dependent Hartree (MCTDH) approach for solving the SchrÃ¶dinger equation with a general potential energy surface. Journal of Chemical Physics, 2018, 148, 044115.	1.2	23

#	Article	IF	Citations
127	A timeâ€dependent calculation of the alignment and orientation of the CN fragment of the photodissociation of ICN. Journal of Chemical Physics, 1996, 105, 141-155.	1.2	22
128	Theoretical and Experimental Study of the Rovibrational Spectrum of He₂â^'CO. Journal of Physical Chemistry A, 2009, 113, 13331-13341.	1.1	22
129	Quenching of NH(bâ€‰1Î£+) by O and N atoms; isotope effect in the quenching of NH and ND(bâ€‰1Î£+) by He, Ar, and N2. Journal of Chemical Physics, 1976, 65, 4940-4944.	1.2	21
130	Parameterized Bases for Calculating Vibrational Spectra Directly from ab Initio Data Using Rectangular Collocation. Journal of Chemical Theory and Computation, 2012, 8, 2053-2061.	2.3	21
131	Assessing the utility of phase-space-localized basis functions: Exploiting direct product structure and a new basis function selection procedure. Journal of Chemical Physics, 2016, 144, 244115.	1.2	21
132	A pruned collocation-based multiconfiguration time-dependent Hartree approach using a Smolyak grid for solving the SchrÃ¶dinger equation with a general potential energy surface. Journal of Chemical Physics, 2019, 150, 154108.	1.2	21
133	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
134	Using a Nondirect Product Basis to Compute J > 0 Rovibrational States of H₃⁺. Journal of Physical Chemistry A, 2013, 117, 9493-9500.	1.1	19
135	Computing vibrational energy levels of CH4 with a Smolyak collocation method. Journal of Chemical Physics, 2017, 147, 144102.	1.2	19
136	Reducing the cost of using collocation to compute vibrational energy levels: Results for CH2NH. Journal of Chemical Physics, 2017, 147, 064103.	1.2	19
137	Computational study of the ro-vibrational spectrum of COâ€“CO2. Journal of Chemical Physics, 2019, 151, 084307.	1.2	19
138	Energy disposal in the photodissociation HCN(Ãƒ1Aâ€³) â†' H + CN(X 2Î£) at 193 nm. Chemical Physics, 1987, 113, 119-130.	0.9	18
139	Mixing quantum-classical molecular dynamics methods applied to intramolecular proton transfer in acetylacetone. Journal of Computational Chemistry, 1997, 18, 1760-1772.	1.5	18
140	Rate constants in quantum mechanical systems: A rigorous and practical path-integral formulation for computer simulations. Chemical Physics Letters, 1998, 293, 209-220.	1.2	18
141	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.	0.4	18
142	Communication: Favorable dimensionality scaling of rectangular collocation with adaptable basis functions up to 7 dimensions. Journal of Chemical Physics, 2013, 139, 051101.	1.2	18
143	Using symmetry-adapted optimized sum-of-products basis functions to calculate vibrational spectra. Chemical Physics Letters, 2016, 644, 183-188.	1.2	18
144	A time-to-energy Fourier resolution method for calculating bound state energies and wavefunctions. Analysis of the method and application to 2D ArHCl. Chemical Physics Letters, 1994, 228, 144-152.	1.2	17

#	Article	IF	Citations
145	Vibrational Levels of Ar4:Â New Odd-Parity Bosonic Statesâ€. Journal of Physical Chemistry A, 2007, 111, 10220-10225.	1.1	17
146	A direct-operation Lanczos approach for calculating energy levels. Chemical Physics Letters, 1996, 257, 98-104.	1.2	16
147	State-to-state and total rotational energy transfer rate constants for CN(Bâ€Š2Î£+,v=0,N)+H2, CN(Xâ€Š2Î£+,v=2,N)+H2, D2, and CN(Xâ€Š2Î£+,v=3,N)+NO. Journal of Chemical Physics, 2002, 116, 3617-3625.	1.2	16
148	Applying a Smolyak collocation method to Cl₂CO. Molecular Physics, 2017, 115, 1775-1785.	0.8	16
149	Reactions of H*(22Pâ€“22S) + H2and their isotopes. Journal of Chemical Physics, 1973, 59, 6035-6051.	1.2	15
150	Photodissociation of HCN at 157â€‚nm: Energy disposal in the CN(Aâ€Š2Î) fragment. Journal of Chemical Physics, 2000, 112, 8904-8909.	1.2	15
151	Computing resonance energies, widths, and wave functions using a Lanczos method in real arithmetic. Journal of Chemical Physics, 2005, 122, 244107.	1.2	15
152	Radiative Recombination of Atoms as a Resonance Scattering Process. Journal of Chemical Physics, 1972, 57, 2033-2037.	1.2	14
153	A Fourier-Lanczos method for calculating energy levels without storing or calculating matrices. Molecular Physics, 1993, 79, 13-23.	0.8	14
154	A direct-operation time-dependent method for calculating absorption spectra involving multiple electronic states and its application to trans-OsO2(oxalate)22â¯. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1999, 55, 575-583.	2.0	14
155	K-independent vibrational bases for systems with large amplitude motion. Molecular Physics, 2012, 110, 825-835.	0.8	14
156	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.	1.3	14
157	Infrared spectrum and intermolecular potential energy surface of the COâ€“O₂ dimer. Physical Chemistry Chemical Physics, 2018, 20, 14431-14440.	1.3	13
158	Perturbation theory for bending potentials. Molecular Physics, 1990, 70, 757-766.	0.8	12
159	A simplified transformation of the rotationalâ€“vibrational Hamiltonian to eliminate a Coriolis term and perturbation theory for higher order terms. Journal of Chemical Physics, 1991, 95, 1884-1899.	1.2	12
160	Quantum canonical transformation of the rotationalâ€“vibrational Hamiltonian to remove a Coriolis term. Journal of Chemical Physics, 1991, 94, 461-477.	1.2	12
161	The advantage of writing kinetic energy operators in polyspherical curvilinear coordinates in terms of zi=cosâ€Šti. Journal of Chemical Physics, 2000, 112, 4413-4414.	1.2	12
162	Machine Learning Optimization of the Collocation Point Set for Solving the Kohnâ€“Sham Equation. Journal of Physical Chemistry A, 2019, 123, 10631-10642.	1.1	12

#	Article	IF	Citations
163	Computational study of the rovibrational spectrum of CO2â€“N2. Physical Chemistry Chemical Physics, 2020, 22, 22674-22683.	1.3	12
164	Collisional Deactivation of H(22P) Fluorescence. Journal of Chemical Physics, 1970, 53, 4244-4248.	1.2	11
165	Comment on â€œSpectral filters in quantum mechanics: A measurement theory perspectiveâ€. Physical Review E, 2002, 65, 028701.	0.8	11
166	Using a nondirect product discrete variable representation for angular coordinates to compute vibrational levels of polyatomic molecules. Journal of Chemical Physics, 2008, 128, 194109.	1.2	11
167	Parallel methods for high-dimensional quantum dynamics. Computer Physics Communications, 2010, 181, 455-461.	3.0	11
168	Nonspectral Methods for Solving the SchrÃ¶dinger Equation for Electronic and Vibrational Problems. Journal of Physical Chemistry Letters, 2011, 2, 2193-2199.	2.1	11
169	Towards Accurate Spectroscopic Identification of Species at Catalytic Surfaces: Anharmonic Vibrations of Formate on AuPt. Materials Research Society Symposia Proceedings, 2012, 1484, 1.	0.1	11
170	Using rectangular collocation with finite difference derivatives to solve electronic SchrÃ¶dinger equation. Journal of Chemical Physics, 2018, 149, 204105.	1.2	11
171	The vibration-rotation-tunneling levels of N2â€“H2O and N2â€“D2O. Journal of Chemical Physics, 2015, 143, 024303.	1.2	10
172	Comparison of different eigensolvers for calculating vibrational spectra using low-rank, sum-of-product basis functions. Molecular Physics, 2017, 115, 1740-1749.	0.8	10
173	A collocation-based multi-configuration time-dependent Hartree method using mode combination and improved relaxation. Journal of Chemical Physics, 2020, 152, 164117.	1.2	10
174	Using collocation to study the vibrational dynamics of molecules. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 248, 119158.	2.0	10
175	A rectangular collocation multi-configuration time-dependent Hartree (MCTDH) approach with time-independent points for calculations on general potential energy surfaces. Journal of Chemical Physics, 2021, 154, 114107.	1.2	10
176	New bands in the ND c 1 Î-a 1 Î” system: spectroscopic constants of the a 1 Î” state. Chemical Physics Letters, 1979, 66, 287-290.	1.2	9
177	Uses of the transit time distribution in kinetic flow systems. International Journal of Chemical Kinetics, 1985, 17, 685-708.	1.0	9
178	Vibronic coupling in square planar complexes of palladium(II) and platinum(II). Chemical Physics, 2006, 329, 90-98.	0.9	9
179	Estimation of rate constants from growth and decay data. International Journal of Chemical Kinetics, 1982, 14, 517-534.	1.0	8
180	Single rotational state preparation and relaxation in CN(X2Î£+, Î½=2). Stimulated emission pumping and laser-induced fluorescence detection. Chemical Physics Letters, 1990, 169, 185-190.	1.2	8

#	Article	IF	Citations
181	Comment on â€œPhase-Space Approach to Solving the Time-Independent SchrÃ¶dinger Equationâ€• Physical Review Letters, 2015, 114, 058901.	2.9	8
182	Using collocation and a hierarchical basis to solve the vibrational SchrÃ¶dinger equation. Journal of Chemical Physics, 2019, 150, 204108.	1.2	8
183	Production of CN(X) in the reaction of fast hydrogen atoms with HCN. Chemical Physics Letters, 1988, 145, 466-470.	1.2	7
184	Energy disposal in CN(A 2Î) produced in the 157 nm photodissociation of C2N2. Chemical Physics Letters, 1996, 261, 651-658.	1.2	7
185	A new approach for determining the time step when propagating with the Lanczos algorithm. Computer Physics Communications, 2010, 181, 1859-1861.	3.0	7
186	Solving the time-dependent Schroedinger equation by discarding high-energy basis functions. Chemical Physics Letters, 2010, 501, 130-133.	1.2	7
187	Theoretical study of the rovibrational spectrum of He₂â€“OCS. Canadian Journal of Chemistry, 2010, 88, 779-786.	0.6	7
188	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.	0.8	7
189	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.	1.2	7
190	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.	1.2	7
191	Photofragmentation of CH3CN at 193 nm: CN fragment energy distribution. Chemical Physics Letters, 1988, 146, 96-100.	1.2	6
192	A variational calculation of vibrational levels of vinyl radical. Journal of Chemical Physics, 2020, 152, 204311.	1.2	6
193	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.	0.4	6
194	Isolated effective Hamiltonians for two nearly degenerate modes coupled by Coriolis and centrifugal terms. Journal of Chemical Physics, 1993, 98, 83-100.	1.2	5
195	Using the symmetric quasiminimal residuals method to accelerate an inexact spectral transform calculation of energy levels and wave functions. Journal of Chemical Physics, 2001, 114, 6485-6486.	1.2	5
196	Computational Study of the Rovibrational Spectra of CH₂D⁺ and CHD₂⁺. Journal of Physical Chemistry A, 2019, 123, 10281-10289.	1.1	5
197	Extracting Functional Dependence from Sparse Data Using Dimensionality Reduction: Application to Potential Energy Surface Construction. Lecture Notes in Computational Science and Engineering, 2011, , 133-149.	0.1	5
198	An adiabatic energy-level expression for anharmonic hydrogen-bonded systems. Molecular Physics, 1990, 71, 1155-1162.	0.8	4

#	Article	IF	Citations
199	Vibrational effects on cross sections for elastic scattering of X-rays and fast electrons by H2O molecules. Chemical Physics Letters, 1993, 207, 407-413.	1.2	4
200	Vibrational polarizabilities of Na3 computed from density functional theory property surfaces and a variational vibrational calculation. Chemical Physics Letters, 1998, 287, 307-314.	1.2	4
201	Energy disposal in CN(Xâ€‰2Î£+) produced in the 157 nm photodissociation of acrylonitrile. Journal of Chemical Physics, 2001, 115, 8411-8417.	1.2	4
202	Using simply contracted basis functions with the Lanczos algorithm to calculate vibrational spectra. International Journal of Quantum Chemistry, 2004, 99, 556-566.	1.0	4
203	Computing vibrational energy levels by solving linear equations using a tensor method with an imposed rank. Journal of Chemical Physics, 2021, 155, 234105.	1.2	4
204	Calculating and assigning rovibrational energy levels of (15N2O)2, (15N14NO)2, 14N2Oâ€“15N2O and 15N14NOâ€“15N2O. Physical Chemistry Chemical Physics, 2013, 15, 19159.	1.3	3
205	Intermolecular vibrations of the CO2â€“CS2 complex: Experiment and theory agree, but understanding remains challenging. Journal of Molecular Spectroscopy, 2016, 330, 188-193.	0.4	3
206	Iterative Methods for Computing Vibrational Spectra. Mathematics, 2018, 6, 13.	1.1	3
207	Using collocation and solutions for a sum-of-product potential to compute vibrational energy levels for general potentials. Chemical Physics Letters, 2021, 781, 138967.	1.2	3
208	Comparing Nested Sequences of Leja and PseudoGauss Points to Interpolate in 1D and Solve the Schroedinger Equation in 9D. Lecture Notes in Computational Science and Engineering, 2018, , 1-17.	0.1	3
209	Efficiently Transforming from Values of a Function on a Sparse Grid to Basis Coefficients. Lecture Notes in Computational Science and Engineering, 2021, , 229-244.	0.1	3
210	Detection of spurious avoided crossings of potential energy curves. Journal of Chemical Physics, 1979, 70, 2958-2961.	1.2	2
211	Effective Hamiltonians for Coriolisâ€coupled nearly degenerate modes: Illustrative examples. Journal of Chemical Physics, 1993, 99, 7529-7543.	1.2	2
212	Uncoupled effective Hamiltonians for molecules with several vibrational modes coupled by Coriolis and centrifugal terms. Chemical Physics, 1997, 219, 31-42.	0.9	2
213	Calculating interior eigenvalues and eigenvectors with an implicitly restarted and a filter diagonalization method. Applied Numerical Mathematics, 2001, 37, 307-317.	1.2	2
214	Calculating intensities using effective Hamiltonians in terms of Coriolis-adapted normal modes. Journal of Chemical Physics, 2005, 122, 034106.	1.2	2
215	Computing vibrational and ro-vibrational spectra of CH5+. AIP Conference Proceedings, 2015, , .	0.3	2
216	Methods for Computing Ro-vibrational Energy Levels. , 2016, , 135-149.		2

#	Article	IF	Citations
217	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
218	Computing vibrationâ€"rotation-tunnelling levels of HOD dimer. Physical Chemistry Chemical Physics, 2019, 21, 3527-3536.	1.3	2
219	Chemiluminescence of the transition state in chemical reactions. Journal of Photochemistry and Photobiology, 1981, 17, 172-173.	0.6	1
220	Rovibrational spectra of molecules in small helium clusters. , 2012, , .		1
221	Using pruned basis sets to compute vibrational spectra. , 2012, , .		1
222	Computing polarizabilities without a Hamiltonian matrix. Chemical Physics Letters, 2012, 524, 96-99.	1.2	1
223	Vibrational energy levels of difluorodioxirane computed with variational and perturbative methods from a hybrid force field. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 119, 107-112.	2.0	1
224	A Comparison of Methods for Determining the Time Step When Propagating with the Lanczos Algorithm. Mathematics, 2019, 7, 1109.	1.1	1
225	Ro-vibrational levels for HF2+: The effect of rotation on vibrational splittings for proton transfer. Journal of Chemical Physics, 2000, 113, 7273-7275.	1.2	0
226	A simple equation including anharmonic effects for the vibrational polarisability of a diatomic molecule. Chemical Physics Letters, 2001, 348, 317-320.	1.2	0
227	Representing potential energy surfaces with neural networks and high dimensional model representations. , 2012, , .		0
228	Tribute to Joel M. Bowman. Journal of Physical Chemistry A, 2013, 117, 6905-6906.	1.1	0
229	The He2-OCS complex: Comparison between theory and experiment. Chemical Physics Letters, 2018, 694, 35-39.	1.2	0
230	Redundant coordinates in quantum mechanics. Chemical Physics, 2018, 515, 336-341.	0.9	0
231	A Parallel Algorithm for Computing the Spectrum of CH $_5^+$. Lecture Notes in Computer Science, 2010, , 109-116.	1.0	0
232	Nonproduct Quadrature Grids: Solving the Vibrational SchrÃ¶dinger Equation in 12d. , 2011, , 1-12.		0