Hans-Dieter Meyer

List of Publications by Year
in descending order

208 papers	14,559 citations	29994 54 h-index	20307 116 g-index
222 all docs	222 docs citations	222 times ranked	4442 citing authors

#	Article	IF	Citations
1	The multiconfiguration time-dependent Hartree (MCTDH) method: a highly efficient algorithm for propagating wavepackets. Physics Reports, 2000, 324, 1-105.	10.3	2,065
2	The multi-configurational time-dependent Hartree approach. Chemical Physics Letters, 1990, 165, 73-78.	1.2	1,678
3	A comparison of different propagation schemes for the time dependent SchrÃ¶dinger equation. Journal of Computational Physics, 1991, 94, 59-80.	1.9	882
4	Quantum molecular dynamics: propagating wavepackets and density operators using the multiconfiguration time-dependent Hartree method. Theoretical Chemistry Accounts, 2003, 109, 251-267.	0.5	500
5	Molecular dynamics of pyrazine after excitation to the S2 electronic state using a realistic 24-mode model Hamiltonian. Journal of Chemical Physics, 1999, 110, 936-946.	1.2	412
6	Variational quantum approaches for computing vibrational energies of polyatomic molecules. Molecular Physics, 2008, 106, 2145-2182.	0.8	402
7	Multilayer multiconfiguration time-dependent Hartree method: Implementation and applications to a Henonâ€“Heiles Hamiltonian and to pyrazine. Journal of Chemical Physics, 2011, 134, 044135.	1.2	296
8	Approaches to the approximate treatment of complex molecular systems by the multiconfiguration time-dependent Hartree method. Journal of Chemical Physics, 1999, 111, 2927-2939.	1.2	243
9	Using the MCTDH wavepacket propagation method to describe multimode non-adiabatic dynamics. International Reviews in Physical Chemistry, 2008, 27, 569-606.	0.9	237
10	Calculation and selective population of vibrational levels with the Multiconfiguration Time-Dependent Hartree (MCTDH) algorithm. Chemical Physics, 2006, 329, 179-192.	0.9	215
11	Full dimensional (15-dimensional) quantum-dynamical simulation of the protonated water dimer. II. Infrared spectrum and vibrational dynamics. Journal of Chemical Physics, 2007, 127, 184303.	1.2	207
12	Relaxation of a system with a conical intersection coupled to a bath: A benchmark 24-dimensional wave packet study treating the environment explicitly. Journal of Chemical Physics, 1998, 109, 3518-3529.	1.2	200
13	Studying molecular quantum dynamics with the multiconfiguration timeâ€dependent Hartree method. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 351-374.	6.2	178
14	Product representation of potential energy surfaces. II. Journal of Chemical Physics, 1998, 109, 3772-3779.	1.2	176
15	Dynamics and Infrared Spectroscopy of the Protonated Water Dimer. Angewandte Chemie - International Edition, 2007, 46, 6918-6921.	7.2	171
16	An efficient and robust integration scheme for the equations of motion of the multiconfiguration time-dependent Hartree (MCTDH) method. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1997, 42, 113-129.	1.0	167
17	Classical models for electronic degrees of freedom: Derivation via spin analogy and application to Fâˆ—+H2â†’F+H2. Journal of Chemical Physics, 1979, 71, 2156.	1.2	155
18	Full-dimensional (15-dimensional) quantum-dynamical simulation of the protonated water dimer. I. Hamiltonian setup and analysis of the ground vibrational state. Journal of Chemical Physics, 2007, 127, 184302.	1.2	145

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19	Few-Boson Dynamics in Double Wells: From Single-Atom to Correlated Pair Tunneling. Physical Review Letters, 2008, 100, 040401.	2.9	134
20	A semiclassical approach to inelastic scattering from solid surfaces and to the Debye-Waller factor. Surface Science, 1981, 104, 117-160.	0.8	128
21	Multistate vibronic interactions in the benzene radical cation. II. Quantum dynamical simulations. Journal of Chemical Physics, 2002, 117, 2657-2671.	1.2	122
22	Computation of vibrational energy levels and eigenstates of fluoroform using the multiconfiguration time-dependent Hartree method. Journal of Chemical Physics, 2008, 129, 224109.	1.2	122
23	All mode dynamics at the conical intersection of an octa-atomic molecule: Multi-configuration time-dependent Hartree (MCTDH) investigation on the butatriene cation. Journal of Chemical Physics, 2001, 115, 2088-2100.	1.2	119
24	Temporary anions - calculation of energy and lifetime by absorbing potentials: the resonance. Journal of Physics B: Atomic, Molecular and Optical Physics, 1998, 31, 4107-4122.	0.6	114
25	Theoretical studies of the tunneling splitting of malonaldehyde using the multiconfiguration time-dependent Hartree approach. Journal of Chemical Physics, 2011, 134, 234307.	1.2	103
26	The transformative complex absorbing potential method: a bridge between complex absorbing potentials and smooth exterior scaling. Journal of Physics B: Atomic, Molecular and Optical Physics, 1998, 31, 2279-2304.	0.6	96
27	Dissipative quantum dynamics of anharmonic oscillators with the multiconfiguration time-dependent Hartree method. Journal of Chemical Physics, 2003, 119, 24-33.	1.2	96
28	A study of the mode-selective transâ€“cis isomerization in HONO using ab initio methodology. Journal of Chemical Physics, 2004, 120, 1306-1317.	1.2	96
29	Full dimensional (15 dimensional) quantum-dynamical simulation of the protonated water-dimer IV: Isotope effects in the infrared spectra of D(D2O)2+, H(D2O)2+, and D(H2O)2+ isotopologues. Journal of Chemical Physics, 2009, 131, 034308.	1.2	95
30	The multigrid POTFIT (MGPF) method: Grid representations of potentials for quantum dynamics of large systems. Journal of Chemical Physics, 2013, 138, 014108.	1.2	95
31	Full dimensional (15-dimensional) quantum-dynamical simulation of the protonated water-dimer III: Mixed Jacobi-valence parametrization and benchmark results for the zero point energy, vibrationally excited states, and infrared spectrum. Journal of Chemical Physics, 2009, 130, 234305.	1.2	93
32	Competition between excitation and electronic decay of short-lived molecular states. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1996, 38, 215-232.	1.0	92
33	Electronic decay of molecular clusters: non-stationary states computed by standard quantum chemistry methods. Chemical Physics Letters, 1999, 303, 413-419.	1.2	88
34	The Ãƒ2E/BÌƒ2B2 Photoelectron Bands of Allene beyond the Linear Coupling Scheme:â€‰ An ab Initio Dynamical Study Including All Fifteen Vibrational Modes. Journal of Physical Chemistry A, 2001, 105, 5567-5576.	1.1	88
35	On the interatomic Coulombic decay in the Ne dimer. Journal of Chemical Physics, 2004, 121, 8393.	1.2	86
36	Manifestation of classical chaos in the statistics of quantum energy levels. Physical Review A, 1986, 33, 4334-4341.	1.0	83

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37	Ultracold few-boson systems in a double-well trap. Physical Review A, 2006, 74, .	1.0	81
38	Correlations in ultracold trapped few-boson systems: Transition from condensation to fermionization. Physical Review A, 2006, 74, .	1.0	77
39	Potential energy surface of the CO2? anion. Physical Chemistry Chemical Physics, 2004, 6, 42.	1.3	74
40	Strong Isotope Effects in the Infrared Spectrum of the Zundel Cation. Angewandte Chemie - International Edition, 2009, 48, 352-355.	7.2	74
41	On the Effect of Initial Rotation on Reactivity. A Multi-Configuration Time-Dependent Hartree (MCTDH) Wave Packet Propagation Study on the H + D2and D + H2Reactive Scattering Systemsâ€. Journal of Physical Chemistry A, 2001, 105, 2604-2611.	1.1	73
42	Optical potentials for electron-molecule scattering: A comparative study on theN2Îg2resonance. Physical Review A, 1989, 40, 5605-5613.	1.0	72
43	A multilayer MCTDH study on the full dimensional vibronic dynamics of naphthalene and anthracene cations. Journal of Chemical Physics, 2013, 138, 014313.	1.2	71
44	On the forced harmonic oscillator with time-dependent frequency. Chemical Physics, 1981, 61, 365-383.	0.9	69
45	Electronic and nuclear motion and their couplings in the presence of a magnetic field. Physical Review A, 1988, 38, 6066-6079.	1.0	69
46	Composite fermionization of one-dimensional Bose-Bose mixtures. Physical Review A, 2008, 78, .	1.0	69
47	Time-dependent rotated hartree approach. Chemical Physics Letters, 1987, 140, 525-530.	1.2	66
48	Dynamics of dissociative attachment of electrons to water through theB12metastable state of the anion. Physical Review A, 2004, 69, .	1.0	60
49	Rotational excitation cross sections of para-H2+para-H2 collisions. A full-dimensional wave-packet propagation study using an exact form of the kinetic energy. Journal of Chemical Physics, 2005, 123, 174311.	1.2	60
50	Tunneling dynamics of a few bosons in a double well. Physical Review A, 2008, 78, .	1.0	60
51	Vibronic Transitions and Quantum Dynamics in Molecular Oligomers: A Theoretical Analysis with an Application to Aggregates of Perylene Bisimides. Journal of Physical Chemistry A, 2009, 113, 13475-13482.	1.1	58
52	Multiphonon energy transfer in atom-surface scattering. Chemical Physics, 1984, 85, 189-200.	0.9	57
53	Time-dependent wave packet study on trans-cis isomerization of HONO. Journal of Chemical Physics, 2004, 120, 6072-6084.	1.2	56
54	Automatic computer procedure for generating exact and analytical kinetic energy operators based on the polyspherical approach. Journal of Chemical Physics, 2012, 136, 034107.	1.2	56

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55	Theoretical study of resonant vibrational excitation ofCO2by electron impact. Physical Review A, 2002, 65, .	1.0	54
56	Resonant vibrational excitation ofCO2by electron impact: Nuclear dynamics on the coupled components of the2Îuresonance. Physical Review A, 2003, 67, .	1.0	54
57	Angularly resolved Auger rates of LiF and HF. Physical Review A, 1992, 46, 5643-5652.	1.0	51
58	Reaction cross sections for the H+D2(Î½0=1)â†'HD+D and D+H2(Î½0=1)â†'DH+H systems. A multiconfiguration time-dependent Hartree (MCTDH) wave packet propagation study. Journal of Chemical Physics, 2002, 116, 10641-10647.	1.2	51
59	Time-dependent interplay between electron emission and fragmentation in the interatomic Coulombic decay. Journal of Chemical Physics, 2003, 118, 2092-2107.	1.2	51
60	Calculation of the vibrational excited states of malonaldehyde and their tunneling splittings with the multi-configuration time-dependent Hartree method. Journal of Chemical Physics, 2014, 141, 034116.	1.2	50
61	MetastableC22â^'Dianion. Physical Review Letters, 1997, 79, 1237-1240.	2.9	49
62	Theoretical study of excitations in furan: Spectra and molecular dynamics. Journal of Chemical Physics, 2004, 121, 4585-4598.	1.2	49
63	Controlled Interplay between Decay and Fragmentation in Resonant Auger Processes. Physical Review Letters, 1998, 80, 1865-1868.	2.9	48
64	Time-dependent wave packet study ontrans-cisisomerization of HONO driven by an external field. Journal of Chemical Physics, 2007, 127, 164315.	1.2	47
65	Molecular scattering wave functions for Auger decay rates: The Auger spectrum of hydrogen fluoride. Physical Review A, 1992, 45, 318-328.	1.0	45
66	A proton between two waters: insight from full-dimensional quantum-dynamics simulations of the [H2Oâ€"Hâ€"OH2]+ cluster. Physical Chemistry Chemical Physics, 2008, 10, 4692.	1.3	44
67	Rotational excitations in para-H2+para-H2 collisions: Full- and reduced-dimensional quantum wave packet studies comparing different potential energy surfaces. Journal of Chemical Physics, 2008, 128, 064305.	1.2	44
68	Benchmark calculations on high-dimensional Henonâ€"Heiles potentials with the multi-configuration time dependent Hartree (MCTDH) method. Journal of Chemical Physics, 2002, 117, 10499-10505.	1.2	43
69	Femtosecond laser pulse control of multidimensional vibrational dynamics: Computational studies on the pyrazine molecule. Journal of Chemical Physics, 2006, 125, 014102.	1.2	43
70	Extracting accurate bound-state spectra from approximate wave packet propagation using the filter-diagonalization method. Journal of Chemical Physics, 1998, 109, 3730-3741.	1.2	41
71	Efficiently computing bound-state spectra: A hybrid approach of the multi-configuration time-dependent Hartree and filter-diagonalization methods. Journal of Chemical Physics, 2001, 114, 2036-2046.	1.2	41
72	Intramolecular vibrational energy redistribution in the highly excited fluoroform molecule: A quantum mechanical study using the multiconfiguration time-dependent Hartree algorithm. Journal of Chemical Physics, 2004, 120, 6992-6998.	1.2	40

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73	Intramolecular vibrational energy redistribution in toluene: a nine-dimensional quantum mechanical study using the MCTDH algorithm. Chemical Physics, 2004, 304, 3-15.	0.9	40
74	Multistate vibronic interactions in difluorobenzene radical cations. II. Quantum dynamical simulations. Journal of Chemical Physics, 2008, 129, 074311.	1.2	40
75	Full dimensional quantum-mechanical simulations for the vibronic dynamics of difluorobenzene radical cation isomers using the multilayer multiconfiguration time-dependent Hartree method. Journal of Chemical Physics, 2012, 137, 134302.	1.2	40
76	On the connection between irregular trajectories and the distribution of quantum level spacings. Journal of Physics A, 1984, 17, L831-L836.	1.6	39
77	Theoretical investigation of intramolecular vibrational energy redistribution in highly excited HFCO. Journal of Chemical Physics, 2006, 124, 194304.	1.2	39
78	A classical model of vibronic coupling: The ultrafast non-radiative decay via a conical intersection. Chemical Physics, 1983, 82, 199-205.	0.9	38
79	Ab initiocalculation of energies and lifetimes of metastable dianions: The C22â^' resonance. Journal of Chemical Physics, 2000, 112, 6635-6642.	1.2	38
80	Interatomic Coulombic decay in a heteroatomic rare gas cluster. Journal of Chemical Physics, 2006, 124, 154305.	1.2	38
81	Excitations of few-boson systems in one-dimensional harmonic and double wells. Physical Review A, 2007, 75, .	1.0	38
82	Rovibrational energy transfer in ortho-H2+para-H2 collisions. Journal of Chemical Physics, 2007, 127, 114310.	1.2	37
83	Schwinger and anomaly-free Kohn variational principles and a generalized Lanczos algorithm for nonsymmetric operators. Physical Review A, 1991, 43, 3587-3596.	1.0	36
84	Multiconfiguration Time-Dependent Hartree Dynamics on an ab Initio Reaction Surface:â€‰ Ultrafast Laser-Driven Proton Motion in Phthalic Acid Monomethylester. Journal of Physical Chemistry A, 2002, 106, 719-724.	1.1	36
85	Exact decay and tunnelling dynamics of interacting few-boson systems. Journal of Physics B: Atomic, Molecular and Optical Physics, 2009, 42, 044018.	0.6	36
86	Transforming high-dimensional potential energy surfaces into sum-of-products form using Monte Carlo methods. Journal of Chemical Physics, 2017, 147, 064105.	1.2	34
87	Reaction cross sections for the H+D2(Î½=0,1) system for collision energies up to 2.5 eV: A multiconfiguration time-dependent Hartree wave-packet propagation study. Journal of Chemical Physics, 1999, 110, 241-248.	1.2	32
88	State filtering by a bath: up to 24 mode numerically exact wavepacket propagations. Chemical Physics Letters, 1999, 299, 451-456.	1.2	32
89	Simulation of a complex spectrum: Interplay of five electronic states and 21 vibrational degrees of freedom in C5H4+. Journal of Chemical Physics, 2005, 123, 204310.	1.2	32
90	On regularizing the MCTDH equations of motion. Journal of Chemical Physics, 2018, 148, 124105.	1.2	32

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91	Calculation of H+H2 and H+D2 reaction probabilities within the multiconfiguration time-dependent Hartree approach employing an adiabatic correction scheme. Journal of Chemical Physics, 1998, 109, 2614-2623.	1.2	31
92	Ab initiostudy of the resonant electron attachment to the F2 molecule. Journal of Chemical Physics, 2002, 117, 10635-10647.	1.2	31
93	Multimode Jahnâ^Teller and Pseudo-Jahnâ^Teller Interactions in the Cyclopropane Radical Cation:â€‰ Complex Vibronic Spectra and Nonradiative Decay Dynamics. Journal of Physical Chemistry A, 2007, 111, 1746-1761.	1.1	31
94	Automatic computer procedure for generating exact and analytical kinetic energy operators based on the polyspherical approach: General formulation and removal of singularities. Journal of Chemical Physics, 2013, 139, 204107.	1.2	31
95	A full-dimensional multilayer multiconfiguration time-dependent Hartree study on the ultraviolet absorption spectrum of formaldehyde oxide. Journal of Chemical Physics, 2014, 141, 124309.	1.2	31
96	On regularizing the ML-MCTDH equations of motion. Journal of Chemical Physics, 2018, 149, 044119.	1.2	31
97	Effect of Light-Induced Conical Intersection on the Photodissociation Dynamics of the D₂⁺ Molecule. Journal of Physical Chemistry A, 2013, 117, 8528-8535.	1.1	30
98	Full-dimensional MCTDH/MGPF study of the ground and lowest lying vibrational states of the bihydroxide complex. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 119, 42-51.	2.0	30
99	All ab initio Auger spectra of HF and LiF: energies, intensities and vibrational shifts and broadenings. Chemical Physics Letters, 1993, 206, 247-252.	1.2	29
100	Evidence for a Resonance State ofH2â^. Physical Review Letters, 1996, 77, 470-473.	2.9	29
101	Photoinduced nonadiabatic dynamics of ethene: Six-dimensional wave packet propagations using two different approximations of the kinetic energy operator. Chemical Physics, 2007, 338, 186-199.	0.9	29
102	Frequency dispersed transient absorption spectra of dissolved perylene: A case study using the density matrix version of the MCTDH method. Chemical Physics, 2008, 347, 152-165.	0.9	27
103	A numerical study on the performance of the multiconfiguration time-dependent Hartree method for density operators. Journal of Chemical Physics, 2000, 112, 10718-10729.	1.2	26
104	A generalised 17-state vibronic-coupling Hamiltonian model for ethylene. Journal of Chemical Physics, 2012, 137, 084304.	1.2	25
105	Rovibrational spectroscopy using a kinetic energy operator in Eckart frame and the multi-configuration time-dependent Hartree (MCTDH) approach. Journal of Chemical Physics, 2014, 141, 114101.	1.2	25
106	Rotational effects on the dissociation dynamics of CHD₃ on Pt(111). Physical Chemistry Chemical Physics, 2016, 18, 8174-8185.	1.3	25
107	In-plane surface scattering in two and three dimensions. Rainbow structure, energy spectra and the influence of surface temperature. Chemical Physics, 1979, 36, 327-344.	0.9	24
108	Vibrational excitons in Î±-helical polypeptides: Multiexciton self-trapping and related infrared transient absorption. Journal of Chemical Physics, 2006, 124, 134907.	1.2	24

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109	Quantum dynamics study of fulvene double bond photoisomerization: The role of intramolecular vibrational energy redistribution and excitation energy. Journal of Chemical Physics, 2011, 135, 134303.	1.2	24
110	Ozone Photodissociation: Isotopic and Electronic Branching Ratios for Symmetric and Asymmetric Isotopologues. Journal of Physical Chemistry A, 2012, 116, 12271-12279.	1.1	24
111	Potential energy curve of the X2Sigmau+resonance state of F2-computed by CAP/CI. Journal of Physics B: Atomic, Molecular and Optical Physics, 1999, 32, L547-L556.	0.6	23
112	Multiconfiguration time-dependent Hartree method applied to molecular dissociation on surfaces: H2+Pt(111). Journal of Chemical Physics, 2006, 124, 074706.	1.2	23
113	Theoretical investigation of highly excited vibrational states in DFCO: Calculation of the out-of-plane bending states and simulation of the intramolecular vibrational energy redistribution. Journal of Chemical Physics, 2007, 126, 024302.	1.2	23
114	Nuclear dynamics during the resonant Auger decay of water molecules. Journal of Chemical Physics, 2009, 130, 154307.	1.2	23
115	Ozone photolysis: Strong isotopologue/isotopomer selectivity in the stratosphere. Journal of Geophysical Research D: Atmospheres, 2014, 119, 4286-4302.	1.2	23
116	The electronic excited states of ethylene with large-amplitude deformations: A dynamical symmetry group investigation. Chemical Physics, 2010, 377, 30-45.	0.9	22
117	Rotational and diffractive inelastic scattering of a diatom on a corrugated surface: A multiconfiguration time-dependent Hartree study on N2/LiF(001). Journal of Chemical Physics, 2001, 114, 1382-1392.	1.2	21
118	Simulating strongly correlated multiparticle systems in a truncated Hilbert space. Physical Review A, 2011, 84, .	1.0	21
119	Numeric kinetic energy operators for molecules in polyspherical coordinates. Journal of Chemical Physics, 2012, 136, 234112.	1.2	21
120	Multidimensional Quantum Mechanical Modeling of Electron Transfer and Electronic Coherence in Plant Cryptochromes: The Role of Initial Bath Conditions. Journal of Physical Chemistry B, 2018, 122, 126-136.	1.2	21
121	Rotational excitation ofN2andCl2molecules by electron impact in the energy range 0.01â€“1000 eV: Investigation of excitation mechanisms. Physical Review A, 1995, 51, 3819-3830.	1.0	20
122	Nonadiabatic Nuclear Dynamics after Valence Ionization of H₂O. Journal of Physical Chemistry A, 2010, 114, 9893-9901.	1.1	20
123	Effect of the overall rotation on the cisâ€“trans isomerization of HONO induced by an external field. Physical Chemistry Chemical Physics, 2012, 14, 3791.	1.3	20
124	Evidence for a metastable state of the fundamental dianionH2â^'. Physical Review A, 1997, 55, 1903-1910.	1.0	19
125	Multiconfigurational expansions of density operators: equations of motion and their properties. Theoretical Chemistry Accounts, 2000, 104, 358-369.	0.5	19
126	Energy Level Statistics of Coupled Oscillators. Physica Scripta, 1987, 35, 125-131.	1.2	18

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127	Photodissociation of the ArHBr complex investigated with the multiconfiguration time-dependent Hartree approach. Journal of Chemical Physics, 2003, 118, 600-609.	1.2	18
128	MULTIDIMENSIONAL DYNAMICS INVOLVING A CONICAL INTERSECTION: WAVEPACKET CALCULATIONS USING THE MCTDH METHOD. Advanced Series in Physical Chemistry, 2004, , 583-617.	1.5	18
129	Proton conduction along a chain of water molecules. Development of a linear model and quantum dynamical investigations using the multiconfiguration time-dependent Hartree method. Journal of Chemical Physics, 2005, 122, 104505.	1.2	18
130	Theoretical investigation of intramolecular vibrational energy redistribution in HFCO and DFCO induced by an external field. Journal of Chemical Physics, 2008, 129, 144304.	1.2	18
131	Multiconfiguration time-dependent Hartree approach to study the OH+H2 reaction. Journal of Chemical Physics, 2010, 132, 214304.	1.2	18
132	Suitable coordinates for quantum dynamics: Applications using the multiconfiguration time-dependent Hartree (MCTDH) algorithm. Computational and Theoretical Chemistry, 2012, 990, 75-89.	1.1	18
133	Inclusion of electron correlation for the target wave function in low-energyeâˆ'+N2scattering. Physical Review A, 1992, 46, 186-193.	1.0	17
134	A hybrid approach of the multi-configuration time-dependent Hartree and filter-diagonalisation methods for computing bound-state spectra. Application to HO2. Physical Chemistry Chemical Physics, 2001, 3, 1576-1582.	1.3	17
135	Computing the energy-dependent width of temporary anions from â„'2ab initiomethods. Journal of Physics B: Atomic, Molecular and Optical Physics, 2002, 35, 1841-1863.	0.6	17
136	Photodissociation of a HCl molecule adsorbed on ice. Chemical Physics Letters, 2005, 406, 202-209.	1.2	17
137	Absorption Cross Section of Ozone Isotopologues Calculated with the Multiconfiguration Time-Dependent Hartree (MCTDH) Method: I. The Hartley and Huggins Bands. Journal of Physical Chemistry A, 2010, 114, 9855-9863.	1.1	17
138	Vertical transition energies vs. absorption maxima: Illustration with the UV absorption spectrum of ethylene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 119, 52-58.	2.0	17
139	A generalised vibronic-coupling Hamiltonian model for benzopyran. Journal of Chemical Physics, 2014, 140, 044301.	1.2	17
140	Atom-triatom rigid rotor inelastic scattering with the MultiConfiguration Time Dependent Hartree approach. Chemical Physics Letters, 2017, 668, 42-46.	1.2	16
141	Quantum dynamics of two bosons in an anharmonic trap: Collective versus internal excitations. Physical Review A, 2007, 76, .	1.0	15
142	Using n-mode potentials for reactive scattering: Application to the 6D H2+Pt(111) problem. Chemical Physics Letters, 2007, 440, 334-340.	1.2	15
143	Interrelation between the Distributions of Kinetic Energy Release and Emitted Electron Energy following the Decay of Electronic States. Physical Review Letters, 2011, 107, 173001.	2.9	15
144	Laser-induced enhancement of tunneling in NHD2. Journal of Chemical Physics, 2012, 136, 194308.	1.2	15

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145	Multidimensional density operator propagations in open systems: Model studies on vibrational relaxations and surface sticking processes. Journal of Chemical Physics, 2004, 121, 9283-9296.	1.2	14
146	Comparison of the Huggins Band for Six Ozone Isotopologues: Vibrational Levels and Absorption Cross Section. Journal of Physical Chemistry A, 2012, 116, 12260-12270.	1.1	14
147	Resonances of HCO Computed Using an Approach Based on the Multiconfiguration Time-Dependent Hartree Method. Journal of Physical Chemistry A, 2015, 119, 12043-12051.	1.1	14
148	On the infrared absorption spectrum of the hydrated hydroxide (<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 632 Td (xmlns:mml= cluster anion. Chemical Physics, 2017, 482, 100-105.	0.9	14
149	Towards a systematic convergence of Multi-Layer (ML) Multi-Configuration Time-Dependent Hartree nuclear wavefunctions: The ML-spawning algorithm. Chemical Physics, 2017, 482, 113-123.	0.9	14
150	Comparison of the multi-layer multi-configuration time-dependent Hartree (ML-MCTDH) method and the density matrix renormalization group (DMRG) for ground state properties of linear rotor chains. Journal of Chemical Physics, 2021, 154, 174106.	1.2	14
151	Inelastic transitions in vibrationally excitedNa2induced by intermediate-energy-electron impact. Physical Review A, 1991, 44, 268-273.	1.0	13
152	Dynamical pruning of the non-equilibrium quantum dynamics of trapped ultracold bosons. Journal of Chemical Physics, 2019, 151, .	1.2	13
153	Novel aspects of ultrafast non-radiative processes. Chemical Physics Letters, 1984, 107, 149-154.	1.2	12
154	Direct calculation of complex resonance poles using separable expansions of the potential: Application to theÎ£u+2shape resonance in electron-H2scattering. Physical Review A, 1986, 33, 222-232.	1.0	12
155	Cross sections and rate constants for OH + H2 reaction on three different potential energy surfaces for ro-vibrationally excited reagents. Journal of Chemical Physics, 2011, 135, 194302.	1.2	12
156	MCTDH study on vibrational states of the CO/Cu(100) system. Journal of Chemical Physics, 2013, 139, 164709.	1.2	12
157	Lattice effects of surface cell: Multilayer multiconfiguration time-dependent Hartree study on surface scattering of CO/Cu(100). Journal of Chemical Physics, 2017, 146, .	1.2	12
158	Improving the mapping mechanism of the mapped Fourier method. Chemical Physics Letters, 2002, 352, 486-490.	1.2	11
159	Cumulative isomerization probability studied by various transition state wave packet methods including the MCTDH algorithm. Benchmark: HCNâ†'CNH isomerization. Journal of Chemical Physics, 2004, 121, 644-654.	1.2	11
160	Wave packet study of the UV photodissociation of the Ar2HBr complex. Journal of Chemical Physics, 2005, 122, 184313.	1.2	11
161	Multiconfiguration time-dependent Hartree and classical dynamics studies of the photodissociation of HF and HCl molecules adsorbed on ice: Extension to three dimensions. Journal of Chemical Physics, 2009, 131, 194303.	1.2	10
162	Fully quantal treatment of nonadiabatic molecular photodynamics: General considerations and application to the benzene cation. Computational and Theoretical Chemistry, 2019, 1150, 71-84.	1.1	10

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163	Regularizing the MCTDH equations of motion through an optimal choice on-the-fly (i.e., spawning) of unoccupied single-particle functions. Journal of Chemical Physics, 2020, 153, 234114.	1.2	10
164	Dynamics of excited molecular states. Journal of Physics: Conference Series, 2005, 4, 66-73.	0.3	9
165	Classical and quantum studies of the photodissociation of a HX (X=Cl,F) molecule adsorbed on ice. Journal of Chemical Physics, 2007, 127, 164717.	1.2	9
166	Importance of Appropriately Regularizing the ML-MCTDH Equations of Motion. Journal of Physical Chemistry A, 2021, 125, 3077-3087.	1.1	9
167	The Multi-Configuration Hartree Approach. , 1993, , 141-152.		8
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