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	Importance of Appropriately Regularizing the ML-MCTDH Equations of Motion. Journal of Physical Chemistry A, 2021, 125, 3077-3087.	1.1	9
2	Localization dynamics in a centrally coupled system. Physical Review B, 2021, 103, .	1.1	3
3	High-Dimensional Quantum Dynamics Study on Excitation-Specific Surface Scattering Including Lattice Effects of a Five-Atom Surface Cell. Journal of Chemical Theory and Computation, 2021, 17, 2702-2713.	2.3	6
4	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
5	Theoretical investigation of the H + HD â†' D + H2 chemical reaction for astrophysical applications: A state-to-state quasi-classical study. Journal of Chemical Physics, 2020, 153, 081102.	1.2	1
6	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
7	Dynamical pruning of the non-equilibrium quantum dynamics of trapped ultracold bosons. Journal of Chemical Physics, 2019, 151, .	1.2	13
8	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
9	Calculation of Global, High-Dimensional Potential Energy Surface Fits in Sum-of-Products Form Using Monte-Carlo Methods. , 2018, , 121-139.		0
10	On regularizing the MCTDH equations of motion. Journal of Chemical Physics, 2018, 148, 124105.	1.2	32
11	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
12	On regularizing the ML-MCTDH equations of motion. Journal of Chemical Physics, 2018, 149, 044119.	1.2	31
13	Atom-triatom rigid rotor inelastic scattering with the MultiConfiguration Time Dependent Hartree approach. Chemical Physics Letters, 2017, 668, 42-46.	1.2	16
14	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
15	Vibronic Couplings. Lecture Notes in Quantum Chemistry II, 2017, , 81-109.	0.3	1
16	Choosing the Set of Coordinates for the Nuclei. Lecture Notes in Quantum Chemistry II, 2017, , 111-125.	0.3	0
17	The Kinetic Energy Operator in Curvilinear Coordinates. Lecture Notes in Quantum Chemistry II, 2017, , 127-166.	0.3	0
18	Introduction to Numerical Methods. Lecture Notes in Quantum Chemistry II, 2017, , 201-285.	0.3	1

#	Article	IF	Citations
19	Photodissociation Spectroscopy. Lecture Notes in Quantum Chemistry II, 2017, , 331-350.	0.3	0
20	Bimolecular Reactions. Lecture Notes in Quantum Chemistry II, 2017, , 351-365.	0.3	0
21	Control of Molecular Processes. Lecture Notes in Quantum Chemistry II, 2017, , 393-424.	0.3	0
22	Group Theory and Molecular Symmetry. Lecture Notes in Quantum Chemistry II, 2017, , 167-199.	0.3	0
23	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
24	On the infrared absorption spectrum of the hydrated hydroxide (<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 552 Td (xmlns:mml= cluster anion. Chemical Physics, 2017, 482, 100-105.	0.9	14
25	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
26	Isotope effects of ground and lowest lying vibrational states of H3â˜'xDxO2â˜' complexes. Journal of Chemical Physics, 2016, 144, 054308.	1.2	4
27	Rotational effects on the dissociation dynamics of CHD₃ on Pt(111). Physical Chemistry Chemical Physics, 2016, 18, 8174-8185.	1.3	25
28	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
29	Expansion Hamiltonian model for a diatomic molecule adsorbed on a surface: Vibrational states of the CO/Cu(100) system including surface vibrations. Journal of Chemical Physics, 2015, 143, 164310.	1.2	8
30	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
31	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
32	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
33	A generalised vibronic-coupling Hamiltonian model for benzopyran. Journal of Chemical Physics, 2014, 140, 044301.	1.2	17
34	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
35	Ozone photolysis: Strong isotopologue/isotopomer selectivity in the stratosphere. Journal of Geophysical Research D: Atmospheres, 2014, 119, 4286-4302.	1.2	23
36	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

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37	Vibrational Spectroscopy and Molecular Dynamics. Physical Chemistry in Action, 2014, , 117-145.	0.1	1
38	Multidimensional Photochemistry Models: Application to Aminobenzonitrile and Benzopyran. , 2014, , .		0
39	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
40	Comparison of the multi-configuration, time-dependent Hartree (MCTDH) method with the Arthurs and Dalgarno coupled-channel method for rotationally inelastic scattering. Chemical Physics Letters, 2013, 585, 184-188.	1.2	5
41	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
42	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
43	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
44	MCTDH study on vibrational states of the CO/Cu(100) system. Journal of Chemical Physics, 2013, 139, 164709.	1.2	12
45	Numerical Studies of the Tunneling Splitting of Malonaldehyde and the Eigenstates of Hydrated Hydroxide Anion Using MCTDH. , 2013, , 201-218.		0
46	Rovibrational energy transfer in collisions of H₂with D₂: a full-dimensional wave packet propagation study. Molecular Physics, 2012, 110, 619-632.	0.8	8
47	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
48	Laser-induced enhancement of tunneling in NHD2. Journal of Chemical Physics, 2012, 136, 194308.	1.2	15
49	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
50	Kinetic energy release in fragmentation processes following electron emission: A time-dependent approach. Journal of Chemical Physics, 2012, 136, 114111.	1.2	4
51	Numeric kinetic energy operators for molecules in polyspherical coordinates. Journal of Chemical Physics, 2012, 136, 234112.	1.2	21
52	Ozone Photodissociation: Isotopic and Electronic Branching Ratios for Symmetric and Asymmetric Isotopologues. Journal of Physical Chemistry A, 2012, 116, 12271-12279.	1.1	24
53	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
54	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

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55	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
56	A generalised 17-state vibronic-coupling Hamiltonian model for ethylene. Journal of Chemical Physics, 2012, 137, 084304.	1.2	25
57	Studying molecular quantum dynamics with the multiconfiguration timeâ€dependent Hartree method. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 351-374.	6.2	178
58	Vibronic Coupling Effects in Resonant Auger Spectra of H₂O. Journal of Physical Chemistry A, 2012, 116, 11140-11150.	1.1	6
59	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
60	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
61	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
62	Simulating strongly correlated multiparticle systems in a truncated Hilbert space. Physical Review A, 2011, 84, .	1.0	21
63	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
64	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
65	Exact decay and tunnelling dynamics of interacting few-boson systems. Journal of Physics B: Atomic, Molecular and Optical Physics, 2010, 43, 029802-029802.	0.6	7
66	The electronic excited states of ethylene with large-amplitude deformations: A dynamical symmetry group investigation. Chemical Physics, 2010, 377, 30-45.	0.9	22
67	Multiconfiguration time-dependent Hartree approach to study the OH+H2 reaction. Journal of Chemical Physics, 2010, 132, 214304.	1.2	18
68	Nonadiabatic Nuclear Dynamics after Valence Ionization of H₂O. Journal of Physical Chemistry A, 2010, 114, 9893-9901.	1.1	20
69	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
70	Distributed Memory Parallelization of the Multi-Configuration Time-Dependent Hartree Method. , 2010, , 147-163.		1
71	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
72	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

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73	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
74	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
75	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
76	Nuclear dynamics during the resonant Auger decay of water molecules. Journal of Chemical Physics, 2009, 130, 154307.	1.2	23
77	Strong Isotope Effects in the Infrared Spectrum of the Zundel Cation. Angewandte Chemie - International Edition, 2009, 48, 352-355.	7.2	74
78	Quantum dynamics through conical intersections in macrosystems: Combining effective modes and time-dependent Hartree. Chemical Physics, 2008, 347, 78-96.	0.9	7
79	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
80	Variational quantum approaches for computing vibrational energies of polyatomic molecules. Molecular Physics, 2008, 106, 2145-2182.	0.8	402
81	Using the MCTDH wavepacket propagation method to describe multimode non-adiabatic dynamics. International Reviews in Physical Chemistry, 2008, 27, 569-606.	0.9	237
82	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
83	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
84	Few-Boson Dynamics in Double Wells: From Single-Atom to Correlated Pair Tunneling. Physical Review Letters, 2008, 100, 040401.	2.9	134
85	Multistate vibronic interactions in difluorobenzene radical cations. II. Quantum dynamical simulations. Journal of Chemical Physics, 2008, 129, 074311.	1.2	40
86	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
87	Composite fermionization of one-dimensional Bose-Bose mixtures. Physical Review A, 2008, 78, .	1.0	69
88	Tunneling dynamics of a few bosons in a double well. Physical Review A, 2008, 78, .	1.0	60
89	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
90	Time-dependent wave packet study ontrans-cisisomerization of HONO driven by an external field. Journal of Chemical Physics, 2007, 127, 164315.	1.2	47

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91	Rovibrational energy transfer in ortho-H2+para-H2 collisions. Journal of Chemical Physics, 2007, 127, 114310.	1.2	37
92	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
93	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
94	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
95	Quantum dynamics of two bosons in an anharmonic trap: Collective versus internal excitations. Physical Review A, 2007, 76, .	1.0	15
96	Excitations of few-boson systems in one-dimensional harmonic and double wells. Physical Review A, 2007, 75, .	1.0	38
97	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
98	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
99	Dynamics and Infrared Spectroscopy of the Protonated Water Dimer. Angewandte Chemie - International Edition, 2007, 46, 6918-6921.	7.2	171
100	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
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	Theoretical investigation of intramolecular vibrational energy redistribution in highly excited HFCO. Journal of Chemical Physics, 2006, 124, 194304.	1.2	39
103	Femtosecond laser pulse control of multidimensional vibrational dynamics: Computational studies on the pyrazine molecule. Journal of Chemical Physics, 2006, 125, 014102.	1.2	43
104	Calculation and selective population of vibrational levels with the Multiconfiguration Time-Dependent Hartree (MCTDH) algorithm. Chemical Physics, 2006, 329, 179-192.	0.9	215
105	On the unphysical impact of complex absorbing potentials on the Hamiltonian and its remedy. Journal of Chemical Physics, 2006, 124, 034102.	1.2	5
106	Multiconfiguration time-dependent Hartree method applied to molecular dissociation on surfaces: H2+Pt(111). Journal of Chemical Physics, 2006, 124, 074706.	1.2	23
107	Vibrational excitons in Î±-helical polypeptides: Multiexciton self-trapping and related infrared transient absorption. Journal of Chemical Physics, 2006, 124, 134907.	1.2	24
108	Correlations in ultracold trapped few-boson systems: Transition from condensation to fermionization. Physical Review A, 2006, 74, .	1.0	77

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109	Ultracold few-boson systems in a double-well trap. Physical Review A, 2006, 74, .	1.0	81
110	Interatomic Coulombic decay in a heteroatomic rare gas cluster. Journal of Chemical Physics, 2006, 124, 154305.	1.2	38
111	Dynamics of excited molecular states. Journal of Physics: Conference Series, 2005, 4, 66-73.	0.3	9
112	The interatomic Coulombic decay in Ne2. Journal of Physics: Conference Series, 2005, 4, 277-281.	0.3	3
113	Multi-electron giant dipole resonances of atoms in crossed electric and magnetic fields. Europhysics Letters, 2005, 71, 373-379.	0.7	4
114	Photodissociation of a HCl molecule adsorbed on ice. Chemical Physics Letters, 2005, 406, 202-209.	1.2	17
115	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
116	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
117	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
118	Wave packet study of the UV photodissociation of the Ar2HBr complex. Journal of Chemical Physics, 2005, 122, 184313.	1.2	11
119	N-electron giant dipole states in crossed electric and magnetic fields. Physical Review A, 2005, 72, .	1.0	2
120	Dynamics of dissociative attachment of electrons to water through theB12metastable state of the anion. Physical Review A, 2004, 69, .	1.0	60
121	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
122	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
123	On the interatomic Coulombic decay in the Ne dimer. Journal of Chemical Physics, 2004, 121, 8393.	1.2	86
124	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
125	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
126	Potential energy surface of the CO2? anion. Physical Chemistry Chemical Physics, 2004, 6, 42.	1.3	74

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127	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
128	Time-dependent wave packet study on trans-cis isomerization of HONO. Journal of Chemical Physics, 2004, 120, 6072-6084.	1.2	56
129	Theoretical study of excitations in furan: Spectra and molecular dynamics. Journal of Chemical Physics, 2004, 121, 4585-4598.	1.2	49
130	MULTIDIMENSIONAL DYNAMICS INVOLVING A CONICAL INTERSECTION: WAVEPACKET CALCULATIONS USING THE MCTDH METHOD. Advanced Series in Physical Chemistry, 2004, , 583-617.	1.5	18
131	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
132	Dissipative quantum dynamics of anharmonic oscillators with the multiconfiguration time-dependent Hartree method. Journal of Chemical Physics, 2003, 119, 24-33.	1.2	96
133	Photodissociation of the ArHBr complex investigated with the multiconfiguration time-dependent Hartree approach. Journal of Chemical Physics, 2003, 118, 600-609.	1.2	18
134	Time-dependent interplay between electron emission and fragmentation in the interatomic Coulombic decay. Journal of Chemical Physics, 2003, 118, 2092-2107.	1.2	51
135	Resonant vibrational excitation ofCO2by electron impact: Nuclear dynamics on the coupled components of the2Îuresonance. Physical Review A, 2003, 67, .	1.0	54
136	Ab initiostudy of the resonant electron attachment to the F2 molecule. Journal of Chemical Physics, 2002, 117, 10635-10647.	1.2	31
137	Theoretical study of resonant vibrational excitation ofCO2by electron impact. Physical Review A, 2002, 65, .	1.0	54
138	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
139	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
140	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
141	Multistate vibronic interactions in the benzene radical cation. II. Quantum dynamical simulations. Journal of Chemical Physics, 2002, 117, 2657-2671.	1.2	122
142	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
143	Improving the mapping mechanism of the mapped Fourier method. Chemical Physics Letters, 2002, 352, 486-490.	1.2	11
144	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

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145	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
146	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
147	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
148	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
149	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
150	Schwingerâ€“Lanczos algorithm for calculation of off-shell -matrix elements and Wynn's epsilon algorithm. Computer Physics Communications, 2000, 131, 41-51.	3.0	6
151	The multiconfiguration time-dependent Hartree (MCTDH) method: a highly efficient algorithm for propagating wavepackets. Physics Reports, 2000, 324, 1-105.	10.3	2,065
152	Multiconfigurational expansions of density operators: equations of motion and their properties. Theoretical Chemistry Accounts, 2000, 104, 358-369.	0.5	19
153	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
154	Ab initiocalculation of energies and lifetimes of metastable dianions: The C22â^' resonance. Journal of Chemical Physics, 2000, 112, 6635-6642.	1.2	38
155	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
156	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
157	Dynamical Greenâ€™s function and an exact optical potential for electron-molecule scattering including nuclear dynamics. Physical Review A, 1999, 60, 2983-2999.	1.0	7
158	Electronic decay of molecular clusters: non-stationary states computed by standard quantum chemistry methods. Chemical Physics Letters, 1999, 303, 413-419.	1.2	88
159	State filtering by a bath: up to 24 mode numerically exact wavepacket propagations. Chemical Physics Letters, 1999, 299, 451-456.	1.2	32
160	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
161	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
162	Theory of wave packet dynamics: resonant Auger spectrum of HF. Journal of Electron Spectroscopy and Related Phenomena, 1998, 93, 17-30.	0.8	6

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163	Product representation of potential energy surfaces. II. Journal of Chemical Physics, 1998, 109, 3772-3779.	1.2	176
164	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
165	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
166	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
167	Controlled Interplay between Decay and Fragmentation in Resonant Auger Processes. Physical Review Letters, 1998, 80, 1865-1868.	2.9	48
168	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
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