# Hans-Dieter Meyer

List of Publications by Year
in descending order



| 208 | 14,559 | 30070 54 | 20358 116 |
|---|---|---|---|
| papers | citations | h-index | g-index |

| 222 | 222 | 222 | 4442 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
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| 1 | The multiconfiguration time-dependent Hartree (MCTDH) method: a highly efficient algorithm for propagating wavepackets. Physics Reports, 2000, 324, 1-105. | 25.6 | 2,065 |
| 2 | The multi-configurational time-dependent Hartree approach. Chemical Physics Letters, 1990, 165, 73-78. | 2.6 | 1,678 |
| 3 | A comparison of different propagation schemes for the time dependent SchrÃ¶dinger equation. Journal of Computational Physics, 1991, 94, 59-80. | 3.8 | 882 |
| 4 | Quantum molecular dynamics: propagating wavepackets and density operators using the multiconfiguration time-dependent Hartree method. Theoretical Chemistry Accounts, 2003, 109, 251-267. | 1.4 | 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. | 3.0 | 412 |
| 6 | Variational quantum approaches for computing vibrational energies of polyatomic molecules. Molecular Physics, 2008, 106, 2145-2182. | 1.7 | 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. | 3.0 | 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. | 3.0 | 243 |
| 9 | Using the MCTDH wavepacket propagation method to describe multimode non-adiabatic dynamics. International Reviews in Physical Chemistry, 2008, 27, 569-606. | 2.3 | 237 |
| 10 | Calculation and selective population of vibrational levels with the Multiconfiguration Time-Dependent Hartree (MCTDH) algorithm. Chemical Physics, 2006, 329, 179-192. | 1.9 | 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. | 3.0 | 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. | 3.0 | 200 |
| 13 | Studying molecular quantum dynamics with the multiconfiguration timeâ€dependent Hartree method. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 351-374. | 14.6 | 178 |
| 14 | Product representation of potential energy surfaces. II. Journal of Chemical Physics, 1998, 109, 3772-3779. | 3.0 | 176 |
| 15 | Dynamics and Infrared Spectroscopy of the Protonated Water Dimer. Angewandte Chemie - International Edition, 2007, 46, 6918-6921. | 13.8 | 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 Fâ^—+H2â†'F+H2. Journal of Chemical Physics, 1979, 71, 2156. | 3.0 | 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. | 3.0 | 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. | 7.8 | 134 |
| 20 | A semiclassical approach to inelastic scattering from solid surfaces and to the Debye-Waller factor. Surface Science, 1981, 104, 117-160. | 1.9 | 128 |
| 21 | Multistate vibronic interactions in the benzene radical cation. II. Quantum dynamical simulations. Journal of Chemical Physics, 2002, 117, 2657-2671. | 3.0 | 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. | 3.0 | 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. | 3.0 | 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. | 1.5 | 114 |
| 25 | Theoretical studies of the tunneling splitting of malonaldehyde using the multiconfiguration time-dependent Hartree approach. Journal of Chemical Physics, 2011, 134, 234307. | 3.0 | 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. | 1.5 | 96 |
| 27 | Dissipative quantum dynamics of anharmonic oscillators with the multiconfiguration time-dependent Hartree method. Journal of Chemical Physics, 2003, 119, 24-33. | 3.0 | 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. | 3.0 | 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. | 3.0 | 95 |
| 30 | The multigrid POTFIT (MGPF) method: Grid representations of potentials for quantum dynamics of large systems. Journal of Chemical Physics, 2013, 138, 014108. | 3.0 | 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. | 3.0 | 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. | 2.6 | 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. | 2.5 | 88 |
| 35 | On the interatomic Coulombic decay in the Ne dimer. Journal of Chemical Physics, 2004, 121, 8393. | 3.0 | 86 |
| 36 | Manifestation of classical chaos in the statistics of quantum energy levels. Physical Review A, 1986, 33, 4334-4341. | 2.5 | 83 |

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| 37 | Ultracold few-boson systems in a double-well trap. Physical Review A, 2006, 74, . | 2.5 | 81 |
| 38 | Correlations in ultracold trapped few-boson systems: Transition from condensation to fermionization. Physical Review A, 2006, 74, . | 2.5 | 77 |
| 39 | Potential energy surface of the CO2? anion. Physical Chemistry Chemical Physics, 2004, 6, 42. | 2.8 | 74 |
| 40 | Strong Isotope Effects in the Infrared Spectrum of the Zundel Cation. Angewandte Chemie - International Edition, 2009, 48, 352-355. | 13.8 | 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. | 2.5 | 73 |
| 42 | Optical potentials for electron-molecule scattering: A comparative study on theN2Îg2resonance. Physical Review A, 1989, 40, 5605-5613. | 2.5 | 72 |
| 43 | A multilayer MCTDH study on the full dimensional vibronic dynamics of naphthalene and anthracene cations. Journal of Chemical Physics, 2013, 138, 014313. | 3.0 | 71 |
| 44 | On the forced harmonic oscillator with time-dependent frequency. Chemical Physics, 1981, 61, 365-383. | 1.9 | 69 |
| 45 | Electronic and nuclear motion and their couplings in the presence of a magnetic field. Physical Review A, 1988, 38, 6066-6079. | 2.5 | 69 |
| 46 | Composite fermionization of one-dimensional Bose-Bose mixtures. Physical Review A, 2008, 78, . | 2.5 | 69 |
| 47 | Time-dependent rotated hartree approach. Chemical Physics Letters, 1987, 140, 525-530. | 2.6 | 66 |
| 48 | Dynamics of dissociative attachment of electrons to water through theB12metastable state of the anion. Physical Review A, 2004, 69, . | 2.5 | 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. | 3.0 | 60 |
| 50 | Tunneling dynamics of a few bosons in a double well. Physical Review A, 2008, 78, . | 2.5 | 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. | 2.5 | 58 |
| 52 | Multiphonon energy transfer in atom-surface scattering. Chemical Physics, 1984, 85, 189-200. | 1.9 | 57 |
| 53 | Time-dependent wave packet study on trans-cis isomerization of HONO. Journal of Chemical Physics, 2004, 120, 6072-6084. | 3.0 | 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. | 3.0 | 56 |

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| 55 | Theoretical study of resonant vibrational excitation ofCO2by electron impact. Physical Review A, 2002, 65, . | 2.5 | 54 |
| 56 | Resonant vibrational excitation ofCO2by electron impact: Nuclear dynamics on the coupled components of the2Îuresonance. Physical Review A, 2003, 67, . | 2.5 | 54 |
| 57 | Angularly resolved Auger rates of LiF and HF. Physical Review A, 1992, 46, 5643-5652. | 2.5 | 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. | 3.0 | 51 |
| 59 | Time-dependent interplay between electron emission and fragmentation in the interatomic Coulombic decay. Journal of Chemical Physics, 2003, 118, 2092-2107. | 3.0 | 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. | 3.0 | 50 |
| 61 | MetastableC22â^'Dianion. Physical Review Letters, 1997, 79, 1237-1240. | 7.8 | 49 |
| 62 | Theoretical study of excitations in furan: Spectra and molecular dynamics. Journal of Chemical Physics, 2004, 121, 4585-4598. | 3.0 | 49 |
| 63 | Controlled Interplay between Decay and Fragmentation in Resonant Auger Processes. Physical Review Letters, 1998, 80, 1865-1868. | 7.8 | 48 |
| 64 | Time-dependent wave packet study ontrans-cisisomerization of HONO driven by an external field. Journal of Chemical Physics, 2007, 127, 164315. | 3.0 | 47 |
| 65 | Molecular scattering wave functions for Auger decay rates: The Auger spectrum of hydrogen fluoride. Physical Review A, 1992, 45, 318-328. | 2.5 | 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. | 2.8 | 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. | 3.0 | 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. | 3.0 | 43 |
| 69 | Femtosecond laser pulse control of multidimensional vibrational dynamics: Computational studies on the pyrazine molecule. Journal of Chemical Physics, 2006, 125, 014102. | 3.0 | 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. | 3.0 | 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. | 3.0 | 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. | 3.0 | 40 |

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| 74 | Multistate vibronic interactions in difluorobenzene radical cations. II. Quantum dynamical simulations. Journal of Chemical Physics, 2008, 129, 074311. | 3.0 | 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. | 3.0 | 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. | 3.0 | 39 |
| 78 | A classical model of vibronic coupling: The ultrafast non-radiative decay via a conical intersection. Chemical Physics, 1983, 82, 199-205. | 1.9 | 38 |
| 79 | Ab initiocalculation of energies and lifetimes of metastable dianions: The C22â^' resonance. Journal of Chemical Physics, 2000, 112, 6635-6642. | 3.0 | 38 |
| 80 | Interatomic Coulombic decay in a heteroatomic rare gas cluster. Journal of Chemical Physics, 2006, 124, 154305. | 3.0 | 38 |
| 81 | Excitations of few-boson systems in one-dimensional harmonic and double wells. Physical Review A, 2007, 75, . | 2.5 | 38 |
| 82 | Rovibrational energy transfer in ortho-H2+para-H2 collisions. Journal of Chemical Physics, 2007, 127, 114310. | 3.0 | 37 |
| 83 | Schwinger and anomaly-free Kohn variational principles and a generalized Lanczos algorithm for nonsymmetric operators. Physical Review A, 1991, 43, 3587-3596. | 2.5 | 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. | 2.5 | 36 |
| 85 | Exact decay and tunnelling dynamics of interacting few-boson systems. Journal of Physics B: Atomic, Molecular and Optical Physics, 2009, 42, 044018. | 1.5 | 36 |
| 86 | Transforming high-dimensional potential energy surfaces into sum-of-products form using Monte Carlo methods. Journal of Chemical Physics, 2017, 147, 064105. | 3.0 | 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. | 3.0 | 32 |
| 88 | State filtering by a bath: up to 24 mode numerically exact wavepacket propagations. Chemical Physics Letters, 1999, 299, 451-456. | 2.6 | 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. | 3.0 | 32 |
| 90 | On regularizing the MCTDH equations of motion. Journal of Chemical Physics, 2018, 148, 124105. | 3.0 | 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. | 3.0 | 31 |
| 92 | Ab initiostudy of the resonant electron attachment to the F2 molecule. Journal of Chemical Physics, 2002, 117, 10635-10647. | 3.0 | 31 |
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| 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. | 3.0 | 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. | 3.0 | 31 |
| 96 | On regularizing the ML-MCTDH equations of motion. Journal of Chemical Physics, 2018, 149, 044119. | 3.0 | 31 |
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| 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. | 3.9 | 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. | 2.6 | 29 |
| 100 | Evidence for a Resonance State ofH2â^. Physical Review Letters, 1996, 77, 470-473. | 7.8 | 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. | 1.9 | 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. | 1.9 | 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. | 3.0 | 26 |
| 104 | A generalised 17-state vibronic-coupling Hamiltonian model for ethylene. Journal of Chemical Physics, 2012, 137, 084304. | 3.0 | 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. | 3.0 | 25 |
| 106 | Rotational effects on the dissociation dynamics of CHD<sub>3</sub> on Pt(111). Physical Chemistry Chemical Physics, 2016, 18, 8174-8185. | 2.8 | 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. | 1.9 | 24 |
| 108 | Vibrational excitons in Î±-helical polypeptides: Multiexciton self-trapping and related infrared transient absorption. Journal of Chemical Physics, 2006, 124, 134907. | 3.0 | 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. | 3.0 | 24 |
| 110 | Ozone Photodissociation: Isotopic and Electronic Branching Ratios for Symmetric and Asymmetric Isotopologues. Journal of Physical Chemistry A, 2012, 116, 12271-12279. | 2.5 | 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. | 1.5 | 23 |
| 112 | Multiconfiguration time-dependent Hartree method applied to molecular dissociation on surfaces: H2+Pt(111). Journal of Chemical Physics, 2006, 124, 074706. | 3.0 | 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. | 3.0 | 23 |
| 114 | Nuclear dynamics during the resonant Auger decay of water molecules. Journal of Chemical Physics, 2009, 130, 154307. | 3.0 | 23 |
| 115 | Ozone photolysis: Strong isotopologue/isotopomer selectivity in the stratosphere. Journal of Geophysical Research D: Atmospheres, 2014, 119, 4286-4302. | 3.3 | 23 |
| 116 | The electronic excited states of ethylene with large-amplitude deformations: A dynamical symmetry group investigation. Chemical Physics, 2010, 377, 30-45. | 1.9 | 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. | 3.0 | 21 |
| 118 | Simulating strongly correlated multiparticle systems in a truncated Hilbert space. Physical Review A, 2011, 84, . | 2.5 | 21 |
| 119 | Numeric kinetic energy operators for molecules in polyspherical coordinates. Journal of Chemical Physics, 2012, 136, 234112. | 3.0 | 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. | 2.6 | 21 |
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| 122 | Nonadiabatic Nuclear Dynamics after Valence Ionization of H<sub>2</sub>O. Journal of Physical Chemistry A, 2010, 114, 9893-9901. | 2.5 | 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. | 2.8 | 20 |
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| 125 | Multiconfigurational expansions of density operators: equations of motion and their properties. Theoretical Chemistry Accounts, 2000, 104, 358-369. | 1.4 | 19 |
| 126 | Energy Level Statistics of Coupled Oscillators. Physica Scripta, 1987, 35, 125-131. | 2.5 | 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. | 3.0 | 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. | 3.0 | 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. | 3.0 | 18 |
| 131 | Multiconfiguration time-dependent Hartree approach to study the OH+H2 reaction. Journal of Chemical Physics, 2010, 132, 214304. | 3.0 | 18 |
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| 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. | 2.8 | 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. | 1.5 | 17 |
| 136 | Photodissociation of a HCl molecule adsorbed on ice. Chemical Physics Letters, 2005, 406, 202-209. | 2.6 | 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. | 2.5 | 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. | 3.9 | 17 |
| 139 | A generalised vibronic-coupling Hamiltonian model for benzopyran. Journal of Chemical Physics, 2014, 140, 044301. | 3.0 | 17 |
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| 141 | Quantum dynamics of two bosons in an anharmonic trap: Collective versus internal excitations. Physical Review A, 2007, 76, . | 2.5 | 15 |
| 142 | Using n-mode potentials for reactive scattering: Application to the 6D H2+Pt(111) problem. Chemical Physics Letters, 2007, 440, 334-340. | 2.6 | 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. | 7.8 | 15 |
| 144 | Laser-induced enhancement of tunneling in NHD2. Journal of Chemical Physics, 2012, 136, 194308. | 3.0 | 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. | 3.0 | 14 |
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| 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. | 2.5 | 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. | 1.9 | 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. | 1.9 | 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. | 3.0 | 14 |
| 151 | Inelastic transitions in vibrationally excitedNa2induced by intermediate-energy-electron impact. Physical Review A, 1991, 44, 268-273. | 2.5 | 13 |
| 152 | Dynamical pruning of the non-equilibrium quantum dynamics of trapped ultracold bosons. Journal of Chemical Physics, 2019, 151, . | 3.0 | 13 |
| 153 | Novel aspects of ultrafast non-radiative processes. Chemical Physics Letters, 1984, 107, 149-154. | 2.6 | 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. | 2.5 | 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. | 3.0 | 12 |
| 156 | MCTDH study on vibrational states of the CO/Cu(100) system. Journal of Chemical Physics, 2013, 139, 164709. | 3.0 | 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, . | 3.0 | 12 |
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