Hans JÃ¸rgen Aagaard Jensen

List of Publications by Year
in descending order

156 papers	11,250 citations	31976 53 h-index	30087 103 g-index
160 all docs	160 docs citations	160 times ranked	5078 citing authors

#	Article	IF	Citations
1	An efficient implementation of time-dependent linear-response theory for strongly orthogonal geminal wave function models. Journal of Chemical Physics, 2022, 156, 174102.	3.0	6
2	Multi-configurational short-range density functional theory can describe spinâ€“spin coupling constants of transition metal complexes. Journal of Chemical Physics, 2021, 155, 084102.	3.0	2
3	Implementation of Relativistic Coupled Cluster Theory for Massively Parallel GPU-Accelerated Computing Architectures. Journal of Chemical Theory and Computation, 2021, 17, 5509-5529.	5.3	17
4	The DIRAC code for relativistic molecular calculations. Journal of Chemical Physics, 2020, 152, 204104.	3.0	191
5	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. Journal of Chemical Physics, 2020, 152, 214115.	3.0	45
6	Remarkable reversal of ¹³C-NMR assignment in d¹, d² compared to d⁸, d⁹ acetylacetonate complexes: analysis and explanation based on solid-state MAS NMR and computations. Physical Chemistry Chemical Physics, 2020, 22, 8048-8059.	2.8	12
7	The Second-Order-Polarization-Propagator-Approximation (SOPPA) in a four-component spinor basis. Journal of Chemical Physics, 2020, 152, 134113.	3.0	16
8	Generalized Valence Bond Perfect-Pairing Made Versatile Through Electron-Pairs Embedding. Journal of Chemical Theory and Computation, 2019, 15, 4430-4439.	5.3	12
9	Triplet excitation energies from multiconfigurational short-range density-functional theory response calculations. Journal of Chemical Physics, 2019, 151, 124113.	3.0	8
10	Relativistic quantum chemical calculations show that the uranium molecule U2 has a quadruple bond. Nature Chemistry, 2019, 11, 40-44.	13.6	72
11	Exploration of H2 binding to the [NiFe]-hydrogenase active site with multiconfigurational density functional theory. Physical Chemistry Chemical Physics, 2018, 20, 794-801.	2.8	17
12	Multiconfigurational short-range density-functional theory for open-shell systems. Journal of Chemical Physics, 2018, 148, 214103.	3.0	35
13	Relativistic Polarizable Embedding. Journal of Chemical Theory and Computation, 2017, 13, 2870-2880.	5.3	14
14	A quantum-mechanical perspective on linear response theory within polarizable embedding. Journal of Chemical Physics, 2017, 146, 234101.	3.0	12
15	Electron correlation within the relativistic no-pair approximation. Journal of Chemical Physics, 2016, 145, 074104.	3.0	41
16	Local electric fields and molecular properties in heterogeneous environments through polarizable embedding. Physical Chemistry Chemical Physics, 2016, 18, 10070-10080.	2.8	60
17	Investigation of Multiconfigurational Short-Range Density Functional Theory for Electronic Excitations in Organic Molecules. Journal of Chemical Theory and Computation, 2016, 12, 2203-2213.	5.3	26
18	Multipole moments for embedding potentials: Exploring different atomic allocation algorithms. Journal of Computational Chemistry, 2016, 37, 1887-1896.	3.3	6

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19	Excitation Spectra of Nucleobases with Multiconfigurational Density Functional Theory. Journal of Physical Chemistry A, 2016, 120, 36-43.	2.5	20
20	Linear interpolation method in ensemble Kohn-Sham and range-separated density-functional approximations for excited states. Physical Review A, 2015, 92, .	2.5	27
21	Beyond the electric-dipole approximation: A formulation and implementation of molecular response theory for the description of absorption of electromagnetic field radiation. Journal of Chemical Physics, 2015, 142, 244111.	3.0	48
22	Polarizable embedding with a multiconfiguration short-range density functional theory linear response method. Journal of Chemical Physics, 2015, 142, 114113.	3.0	29
23	Molecular quantum mechanical gradients within the polarizable embedding approachâ€"Application to the internal vibrational Stark shift of acetophenone. Journal of Chemical Physics, 2015, 142, 034119.	3.0	17
24	Theoretical study on ThF⁺, a prospective system in search of time-reversal violation. New Journal of Physics, 2015, 17, 043005.	2.9	33
25	Density matrix renormalization group with efficient dynamical electron correlation through range separation. Journal of Chemical Physics, 2015, 142, 224108.	3.0	86
26	Performance of SOPPA-based methods in the calculation of vertical excitation energies and oscillator strengths. Molecular Physics, 2015, 113, 2026-2045.	1.7	31
27	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	14.6	1,166
28	Polarizable embedding based on multiconfigurational methods: Current developments and the road ahead. International Journal of Quantum Chemistry, 2014, 114, 1102-1107.	2.0	13
29	Failures of TDDFT in describing the lowest intramolecular charge-transfer excitation in para-nitroaniline. Molecular Physics, 2013, 111, 1235-1248.	1.7	79
30	Alternative separation of exchange and correlation energies in range-separated density-functional perturbation theory. Physical Review A, 2013, 88, .	2.5	16
31	A Unified Framework for the Polarizable Embedding and Continuum Methods Within Multiconfigurational Self-consistent Field Theory. Advances in Quantum Chemistry, 2013, 66, 195-238.	0.8	12
32	Gauge origin independent calculations of molecular magnetisabilities in relativistic four-component theory. Molecular Physics, 2013, 111, 1373-1381.	1.7	28
33	Multi-configuration time-dependent density-functional theory based on range separation. Journal of Chemical Physics, 2013, 138, 084101.	3.0	88
34	Correlated four-component EPR g-tensors for doublet molecules. Journal of Chemical Physics, 2013, 138, 214106.	3.0	21
35	Assessment of charge-transfer excitations with time-dependent, range-separated density functional theory based on long-range MP2 and multiconfigurational self-consistent field wave functions. Journal of Chemical Physics, 2013, 139, 184308.	3.0	39
36	The multi-configuration self-consistent field method within a polarizable embedded framework. Journal of Chemical Physics, 2013, 139, 044101.	3.0	46

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37	Molecular-Level Insight into the Spectral Tuning Mechanism of the DsRed Chromophore. Journal of Physical Chemistry Letters, 2012, 3, 3513-3521.	4.6	54
38	A multiconfigurational hybrid density-functional theory. Journal of Chemical Physics, 2012, 137, 044104.	3.0	77
39	Spinâ€“orbit coupling in actinide cations. Chemical Physics Letters, 2012, 546, 58-62.	2.6	31
40	On the importance of excited state dynamic response electron correlation in polarizable embedding methods. Journal of Computational Chemistry, 2012, 33, 2012-2022.	3.3	38
41	Phosphorescence parameters for platinum (II) organometallic chromophores: A study at the non-collinear four-component Kohnâ€“Sham level of theory. Chemical Physics Letters, 2012, 531, 229-235.	2.6	10
42	Analysis of self-consistency effects in range-separated density-functional theory with MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2011, 135, 034116.	3.0	12
43	Accurate calculations of the ground state and low-lying excited states of the (RbBa)⁺molecular ion: a proposed system for ultracold reactive collisions. Journal of Physics B: Atomic, Molecular and Optical Physics, 2010, 43, 055101.	1.5	14
44	Merging multireference perturbation and density-functional theories by means of range separation: Potential curves for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Be</mml:mi><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>,<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Mg</mml:mi><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></m.	2.5	60
45	Large-scale parallel configuration interaction. II. Two- and four-component double-group general active space implementation with application to BiH. Journal of Chemical Physics, 2010, 132, 014108.	3.0	84
46	On the universality of the long-/short-range separation in multiconfigurational density-functional theory. II. Investigating f actinide species. Journal of Chemical Physics, 2009, 131, 054107.	3.0	49
47	Gauge origin independent calculations of nuclear magnetic shieldings in relativistic four-component theory. Journal of Chemical Physics, 2009, 131, 124119.	3.0	60
48	Modeling enzymatic transition states by force field methods. International Journal of Quantum Chemistry, 2009, 109, 373-383.	2.0	2
49	Relativistic adiabatic timeâ€dependent density functional theory using hybrid functionals and noncollinear spin magnetization. International Journal of Quantum Chemistry, 2009, 109, 2091-2112.	2.0	87
50	Large-scale parallel configuration interaction. I. Nonrelativistic and scalar-relativistic general active space implementation with application to (Rbâ€“Ba)+. Journal of Chemical Physics, 2008, 128, 014108.	3.0	47
51	Self-consistent many-body perturbation theory in range-separated density-functional theory: A one-electron reduced-density-matrix-based formulation. Physical Review A, 2008, 78, .	2.5	56
52	A direct relativistic four-component multiconfiguration self-consistent-field method for molecules. Journal of Chemical Physics, 2008, 129, 034109.	3.0	72
53	Relativistic effects in the intermolecular interaction-induced nuclear magnetic resonance parameters of xenon dimer. Journal of Chemical Physics, 2007, 127, 164313.	3.0	36
54	On the universality of the long-/short-range separation in multiconfigurational density-functional theory. Journal of Chemical Physics, 2007, 126, 074111.	3.0	171

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55	Can Electron Propagator Methods Be Used To Improve Polarization Propagator Methods?. AIP Conference Proceedings, 2007, , .	0.4	0
56	Determination of the chemical potential and HOMO/LUMO orbitals in density purification methods. Chemical Physics Letters, 2006, 432, 591-594.	2.6	8
57	Rotationalgfactors calculated for diatomic molecular cations H2+, HeH+and NeH+. Journal of Physics B: Atomic, Molecular and Optical Physics, 2006, 39, 5215-5223.	1.5	1
58	The generalized active space concept for the relativistic treatment of electron correlation. III. Large-scale configuration interaction and multiconfiguration self-consistent-field four-component methods with application to UO2. Journal of Chemical Physics, 2006, 124, 104106.	3.0	111
59	Quantum-Chemical Calculations of Radial Functions for Rotational and Vibrational g Factors, Electric Dipolar Moment and Adiabatic Corrections to the Potential Energy for Analysis of Spectra of HeH+. Advances in Quantum Chemistry, 2005, , 319-334.	0.8	17
60	Analysis of Pure Rotational and Vibration-rotational Spectra of NaCl X1Î£+and Quantum-chemical Calculation of Related Molecular Properties. Journal of the Chinese Chemical Society, 2005, 52, 631-639.	1.4	4
61	First-order MP2 molecular properties in a relativistic framework. Chemical Physics, 2005, 311, 81-95.	1.9	30
62	Theoretical study of PbO and the PbO anion. Chemical Physics Letters, 2005, 408, 210-215.	2.6	86
63	Two-photon absorption in the relativistic four-component Hartreeâ€“Fock approximation. Journal of Chemical Physics, 2005, 122, 114106.	3.0	15
64	Nonlinear response theory with relaxation: The first-order hyperpolarizability. Journal of Chemical Physics, 2005, 123, 194103.	3.0	178
65	Quadratic response functions in the time-dependent four-component Hartree-Fock approximation. Journal of Chemical Physics, 2004, 121, 6145-6154.	3.0	23
66	Linear response at the 4-component relativistic level: Application to the frequency-dependent dipole polarizabilities of the coinage metal dimers. Journal of Chemical Physics, 2003, 118, 522-536.	3.0	118
67	The tetrathiafulvalene dication in the gas phase: its formation and stability. Physical Chemistry Chemical Physics, 2003, 5, 1376.	2.8	14
68	Relativistic effects on linear and nonlinear polarizabilities studied by effective-core potential, Douglasâ€“Kroll, and Diracâ€“Hartreeâ€“Fock response theory. Journal of Chemical Physics, 2002, 116, 6914-6923.	3.0	60
69	Near-resonant absorption in the time-dependent self-consistent field and multiconfigurational self-consistent field approximations. Journal of Chemical Physics, 2001, 115, 10323.	3.0	197
70	Propagator Calculations of Electronic Spectra of Photochromic Spirooxazines. Molecular Crystals and Liquid Crystals, 2000, 345, 89-94.	0.3	1
71	An investigation of basis set effects in the characterization of electron - atom scattering resonances using the dilated electron propagator method. Theoretical Chemistry Accounts, 2000, 104, 445-454.	1.4	22
72	Ab initiocalculations of molecular resonant photoemission spectra. Journal of Chemical Physics, 2000, 113, 7790-7798.	3.0	26

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73	Relativistic four-component calculations of indirect nuclear spinâ€“spin couplings in MH4 (M=C,â€ŠSi,â€ŠGe,â€ŠSn,â€ŠPb) and Pb(CH3)3H. Journal of Chemical Physics, 2000, 112, 3493-3498.	3.0	96
74	2,2â€˜-Bithiophene Radical Cation:Â An Experimental and Computational Study. Journal of Physical Chemistry A, 2000, 104, 2808-2823.	2.5	26
75	Quaternion symmetry of the Dirac equation. Lecture Notes in Quantum Chemistry II, 2000, , 227-246.	0.3	2
76	Quaternion symmetry in relativistic molecular calculations: The Diracâ€“Hartreeâ€“Fock method. Journal of Chemical Physics, 1999, 111, 6211-6222.	3.0	150
77	On the origin and contribution of the diamagnetic term in four-component relativistic calculations of magnetic properties. Journal of Chemical Physics, 1999, 110, 6208-6218.	3.0	198
78	Generalized integral-screening for efficient calculations of nonlinear optical properties of large molecules. Journal of Chemical Physics, 1998, 108, 7973-7979.	3.0	16
79	Spin-orbit corrections to the indirect nuclear spin-spin coupling constants in XH4 (X = C, Si, Ge, and) Tj ETQq1 1 0.784314 rgBT /Over	0.8	12
80	Spinâ€“orbit corrections to the indirect nuclear spinâ€“spin coupling constants in XH. Theoretica Chimica Acta, 1997, 95, 35.	0.8	34
81	A new implementation of the secondâ€order polarization propagator approximation (SOPPA): The excitation spectra of benzene and naphthalene. Journal of Chemical Physics, 1996, 105, 5886-5900.	3.0	174
82	Relativistic fourâ€component multiconfigurational selfâ€consistentâ€field theory for molecules: Formalism. Journal of Chemical Physics, 1996, 104, 4083-4097.	3.0	121
83	Screening in resonant X-ray emission of molecules. Journal of Electron Spectroscopy and Related Phenomena, 1996, 82, 125-134.	1.7	23
84	Operator representations in Kramers bases. Chemical Physics Letters, 1995, 232, 47-53.	2.6	27
85	Multiconfigurational selfâ€consistent reaction field theory for nonequilibrium solvation. Journal of Chemical Physics, 1995, 103, 9010-9023.	3.0	103
86	Relativistic corrections to molecular dynamic dipole polarizabilities. Journal of Chemical Physics, 1995, 103, 2983-2990.	3.0	13
87	A multiconfiguration selfâ€consistent reaction field response method. Journal of Chemical Physics, 1994, 100, 6597-6607.	3.0	146
88	Multiconfigurational selfâ€consistent field calculations of nuclear shieldings using London atomic orbitals. Journal of Chemical Physics, 1994, 100, 8178-8185.	3.0	229
89	MCSCF reaction-path energetics and thermal rate-constants for the reaction of3NH with H2. Theoretica Chimica Acta, 1994, 89, 157-168.	0.8	6
90	The Vegard-Kaplan band and the phosphorescent decay of N2. Chemical Physics Letters, 1994, 231, 387-394.	2.6	8

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91	Direct one-index transformations in multiconfiguration response calculations. Journal of Computational Chemistry, 1994, 15, 573-579.	3.3	3
92	Correlated calculations of indirect nuclear spin-spin coupling constants for XH4 (X = Si, Ge, and Sn). Chemical Physics, 1994, 188, 171-181.	1.9	72
93	Frequencyâ€dependent polarizabilities of O2 and van der Waals coefficients of dimers containing O2. Journal of Chemical Physics, 1994, 100, 1297-1302.	3.0	48
94	Basis set convergence of atomic axial tensors obtained from selfâ€consistent field calculations using London atomic orbitals. Journal of Chemical Physics, 1994, 100, 6620-6627.	3.0	28
95	Electron Correlation in Molecules Using Direct Second Order MCSCF. NATO ASI Series Series B: Physics, 1994, , 179-206.	0.2	10
96	The nuclear spinâ€”spin coupling in N2 and CO. Chemical Physics Letters, 1993, 209, 201-206.	2.6	38
97	Nuclear magnetic shielding tensor for the ethylenic carbon atom in tetrachlorocyclopropene. Chemical Physics Letters, 1993, 204, 608-610.	2.6	9
98	Large scale random phase calculations for direct self-consistent field wavefunctions. Chemical Physics, 1993, 172, 13-20.	1.9	29
99	Relaxation and correlation contributions to molecular double core ionization energies. Chemical Physics, 1993, 172, 45-57.	1.9	72
100	Gaugeâ€origin independent multiconfigurational selfâ€consistentâ€field theory for vibrational circular dichroism. Journal of Chemical Physics, 1993, 98, 8873-8887.	3.0	186
101	Multiconfiguration linear-response approaches to the calculation of absolute photoionization cross sections: HF,H2O, and Ne. Physical Review A, 1993, 47, 3810-3823.	2.5	25
102	Hartreeâ€“Fock limit magnetizabilities from London orbitals. Journal of Chemical Physics, 1993, 99, 3847-3859.	3.0	202
103	Spin polarization in restricted electronic structure theory: Multiconfiguration selfâ€consistentâ€field calculations of hyperfine coupling constants. Journal of Chemical Physics, 1992, 97, 3412-3419.	3.0	46
104	Spinâ€“orbit coupling constants in a multiconfiguration linear response approach. Journal of Chemical Physics, 1992, 96, 2118-2126.	3.0	90
105	Firstâ€order nonadiabatic coupling matrix elements from multiconfigurational selfâ€consistentâ€field response theory. Journal of Chemical Physics, 1992, 97, 7573-7584.	3.0	31
106	Multiconfigurational quadratic response functions for singlet and triplet perturbations: The phosphorescence lifetime of formaldehyde. Journal of Chemical Physics, 1992, 97, 9178-9187.	3.0	148
107	Interconversion of diborane (4) isomers. Journal of Chemical Physics, 1992, 97, 1211-1216.	3.0	33
108	Quadratic response functions for a multiconfigurational selfâ€consistent field wave function. Journal of Chemical Physics, 1992, 97, 1174-1190.	3.0	209

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109	Indirect nuclear spinâ€“spin coupling constants from multiconfiguration linear response theory. Journal of Chemical Physics, 1992, 96, 6120-6125.	3.0	147
110	The second-order energy contribution from the spin-orbit interaction operator to the potential energy curve of Cr2. International Journal of Quantum Chemistry, 1992, 41, 729-731.	2.0	5
111	Ab initio potential energy function and geometry of the state of ammonia. Journal of Molecular Spectroscopy, 1992, 152, 199-204.	1.2	2
112	Solvatochromatic shifts studied by multi-configuration self-consistent reaction field theory. Application to azabenzenes. Chemical Physics, 1992, 159, 211-225.	1.9	36
113	Frequency-dependent hyperpolarizability of hydrogen fluoride. Chemical Physics Letters, 1992, 191, 293-298.	2.6	42
114	The magnetic hyperpolarizability anisotropy of the neon atom. Chemical Physics Letters, 1992, 191, 599-602.	2.6	17
115	Excited state structures and vibronic spectra of H2CO+, HDCO+, and D2CO+ using molecular gradient and Hessian techniques. Journal of Chemical Physics, 1991, 95, 5906-5917.	3.0	14
116	An ab initio investigation of the potential energy function and rotationâ€”vibration energies of H2OÂ·Na+. Chemical Physics Letters, 1991, 185, 265-269.	2.6	7
117	The hyperpolarizability dispersion of neon is not anomalous. Chemical Physics Letters, 1991, 187, 387-390.	2.6	37
118	Restricted and complete-active-space multiconfiguration linear response calculations of the polarizability of formamide and urea. Chemical Physics Letters, 1991, 186, 379-385.	2.6	12
119	MCSCF/MCLRStudies of potential energy surfaces, spectra, and properties of theX1A1anda3B2states of ozone. International Journal of Quantum Chemistry, 1991, 40, 475-490.	2.0	28
120	Excitation energies from the coupled cluster singles and doubles linear response function (CCSDLR). Applications to Be, CH+, CO, and H2O. Journal of Chemical Physics, 1990, 93, 3345-3350.	3.0	529
121	Integration of the classical equations of motion on ab initio molecular potential energy surfaces using gradients and Hessians: application to translational energy release upon fragmentation. Chemical Physics Letters, 1990, 173, 145-150.	2.6	254
122	Dipole polarizability surfaces of ammonia. Chemical Physics, 1990, 144, 343-351.	1.9	9
123	Coupled cluster energy derivatives. Analytic Hessian for the closedâ€shell coupled cluster singles and doubles wave function: Theory and applications. Journal of Chemical Physics, 1990, 92, 4924-4940.	3.0	222
124	SIRIUS: A General Purpose Direct Second Order MCSCF Program. , 1990, , 435-531.		14
125	Accurate static and dynamic polarizabilities ofLiâ^'. Physical Review A, 1989, 40, 2265-2269.	2.5	30
126	Accurate photodetachment cross sections for Li-. Journal of Physics B: Atomic, Molecular and Optical Physics, 1989, 22, 2133-2140.	1.5	18

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127	Accurate calculations of the dynamic dipole polarizability of N2. A multiconfigurational linear response study using restricted active space (RAS) wavefunctions. Chemical Physics Letters, 1989, 162, 355-360.	2.6	22
128	Excitation energies, transition moments and dynamic polarizabilities for CH+. A comparison of multiconfigurational linear response and full configuration interaction calculations. Chemical Physics Letters, 1989, 154, 380-386.	2.6	107
129	An efficient method for calculating molecular radiative intensities in the VUV and soft X-ray wavelength regions. Physica Scripta, 1989, 40, 745-750.	2.5	45
130	Selfâ€consistent reaction field calculations of photoelectron binding energies for solvated molecules. Journal of Chemical Physics, 1989, 90, 6422-6435.	3.0	40
131	SIRIUS: A General Purpose Direct Second Order MCSCF Program. , 1989, , 577-587.		2
132	Solution of the large matrix equations which occur in response theory. Journal of Computational Physics, 1988, 74, 265-282.	3.8	180
133	On the validity of the equivalent core approximation in Born-Haber analyses of liquids and solutions. Chemical Physics Letters, 1988, 153, 322-327.	2.6	17
134	A gradient extremal walking algorithm. Theoretica Chimica Acta, 1988, 73, 55-65.	0.8	69
135	Determinant based configuration interaction algorithms for complete and restricted configuration interaction spaces. Journal of Chemical Physics, 1988, 89, 2185-2192.	3.0	941
136	A multiconfigurational selfâ€consistent reactionâ€field method. Journal of Chemical Physics, 1988, 89, 3086-3095.	3.0	198
137	Secondâ€order Mo/llerâ€“Plesset perturbation theory as a configuration and orbital generator in multiconfiguration selfâ€consistent field calculations. Journal of Chemical Physics, 1988, 88, 3834-3839.	3.0	176
138	Linear response calculations for large scale multiconfiguration selfâ€consistent field wave functions. Journal of Chemical Physics, 1988, 89, 3654-3661.	3.0	216
139	Efficient optimization of large scale MCSCF wave functions with a restricted step algorithm. Journal of Chemical Physics, 1987, 87, 451-466.	3.0	112
140	Ground-state potential energy surface of diazene. Journal of the American Chemical Society, 1987, 109, 2895-2901.	13.7	66
141	An efficient method for the calculation of generalized overlap amplitudes for core photoelectron shake-up spectra. Chemical Physics Letters, 1987, 137, 431-436.	2.6	31
142	Analytical calculation of MCSCF dipoleâ€moment derivatives. Journal of Chemical Physics, 1986, 84, 6280-6284.	3.0	43
143	A diabatic model for photoionization. Application to the inner valence xâ€ray photoelectron spectrum of acetylene. Journal of Chemical Physics, 1986, 85, 6270-6275.	3.0	14
144	Systematic determination of MCSCF equilibrium and transition structures and reaction paths. Journal of Chemical Physics, 1986, 85, 3917-3929.	3.0	29

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145	A direct, restricted-step, second-order MC SCF program for large scale ab initio calculations. Chemical Physics, 1986, 104, 229-250.	1.9	130
146	Molecular Hessians for largeâ€scale MCSCF wave functions. Journal of Chemical Physics, 1986, 84, 6266-6279.	3.0	109
147	Evaluation of first- and second-order nonadiabatic coupling elements from large multiconfigurational self-consistent-field wave functions. Physical Review A, 1986, 34, 4606-4614.	2.5	19
148	Direct Methods in the Calculation of Analytical Derivatives of Energy Surfaces and Molecular Properties. , 1986, , 215-227.		1
149	Direct restricted-step MCSCF calculations on the structure and spectrum of cyclobutadiene. International Journal of Quantum Chemistry, 1985, 28, 237-246.	2.0	0
150	Polarization propagator calculations with an AGP reference state. Journal of Chemical Physics, 1984, 80, 2009-2021.	3.0	29
151	A direct approach to secondâ€order MCSCF calculations using a norm extended optimization scheme. Journal of Chemical Physics, 1984, 80, 1204-1214.	3.0	101
152	MC SCF optimization using the direct, restricted step, second-order norm-extended optimization method. Chemical Physics Letters, 1984, 110, 140-144.	2.6	95
153	Accurate Hartreeâ€“Fock wave functions without exponent optimization. Journal of Chemical Physics, 1984, 80, 840-855.	3.0	52
154	AGPPropagator calculations. International Journal of Quantum Chemistry, 1983, 23, 65-70.	2.0	14
155	The polarization propagator based on an agp state: Theory and application to the helium atom. International Journal of Quantum Chemistry, 1983, 24, 415-423.	2.0	0
156	A powerful procedure for optimizing AGP states. International Journal of Quantum Chemistry, 1982, 22, 615-631.	2.0	1