Ove Christiansen

List of Publications by Year
in descending order

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206	15,321	15466 65	19136 118
papers	citations	h-index	g-index

207	207	207	6639
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Vibrational Coupled Cluster Theory. , 2022, , 41-79.		1
2	Calculating vibrational excitation energies using tensor-decomposed vibrational coupled-cluster response theory. Journal of Chemical Physics, 2021, 154, 054113.	1.2	3
3	Quantum embedding description of the Anderson lattice model with the ghost Gutzwiller approximation. Physical Review B, 2021, 104, .	1.1	11
4	Bypassing the computational bottleneck of quantum-embedding theories for strong electron correlations with machine learning. Physical Review Research, 2021, 3, .	1.3	5
5	Extended vibrational coupled cluster: Stationary states and dynamics. Journal of Chemical Physics, 2020, 153, 044133.	1.2	9
6	A Gaussian process regression adaptive density guided approach for potential energy surface construction. Journal of Chemical Physics, 2020, 153, 064105.	1.2	17
7	Time-dependent vibrational coupled cluster with variationally optimized time-dependent basis sets. Journal of Chemical Physics, 2020, 153, 174108.	1.2	10
8	Vibrational Coupled Cluster Computations in Polyspherical Coordinates with the Exact Analytical Kinetic Energy Operator. Journal of Chemical Theory and Computation, 2020, 16, 4505-4520.	2.3	8
9	MR-MCTDH[n]: Flexible Configuration Spaces and Nonadiabatic Dynamics within the MCTDH[n] Framework. Journal of Chemical Theory and Computation, 2020, 16, 4087-4097.	2.3	10
10	Toward Accurate Theoretical Vibrational Spectra: A Case Study for Maleimide. Journal of Physical Chemistry A, 2020, 124, 2616-2627.	1.1	8
11	Systematic and variational truncation of the configuration space in the multiconfiguration time-dependent Hartree method: The MCTDH[n] hierarchy. Journal of Chemical Physics, 2020, 152, 084101.	1.2	13
12	Adaptive density-guided approach to double incremental potential energy surface construction. Journal of Chemical Physics, 2020, 152, 194105.	1.2	5
13	Vibrationally resolved coupled-cluster x-ray absorption spectra from vibrational configuration interaction anharmonic calculations. Journal of Chemical Physics, 2020, 153, 234111.	1.2	8
14	A general implementation of time-dependent vibrational coupled-cluster theory. Journal of Chemical Physics, 2020, 153, 234109.	1.2	6
15	Vibrationally resolved emission spectra of luminescent conjugated oligothiophenes from anharmonic calculations. Physical Chemistry Chemical Physics, 2019, 21, 17410-17422.	1.3	15
16	Machine learning for potential energy surfaces: An extensive database and assessment of methods. Journal of Chemical Physics, 2019, 150, 244113.	1.2	42
17	Time-dependent vibrational coupled cluster theory: Theory and implementation at the two-mode coupling level. Journal of Chemical Physics, 2019, 151, 154116.	1.2	16
18	Approximate high mode coupling potentials using Gaussian process regression and adaptive density guided sampling. Journal of Chemical Physics, 2019, 150, 131102.	1.2	36

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19	Assessment of the overlap metric in the context of RI-MP2 and atomic batched tensor decomposed MP2. Chemical Physics Letters, 2018, 701, 7-14.	1.2	3
20	Employing general fit-bases for construction of potential energy surfaces with an adaptive density-guided approach. Journal of Chemical Physics, 2018, 148, 064113.	1.2	23
21	Tensor-decomposed vibrational coupled-cluster theory: Enabling large-scale, highly accurate vibrational-structure calculations. Journal of Chemical Physics, 2018, 148, 024103.	1.2	17
22	Anharmonic vibrational spectra from double incremental potential energy and dipole surfaces. Physical Chemistry Chemical Physics, 2018, 20, 3445-3456.	1.3	20
23	Gaussian process regression to accelerate geometry optimizations relying on numerical differentiation. Journal of Chemical Physics, 2018, 148, 241704.	1.2	54
24	Describing Molecules in Motion by Quantum Many-Body Methods. , 2018, , 199-221.		0
25	Exponential parameterization of wave functions for quantum dynamics: Time-dependent Hartree in second quantization. Journal of Chemical Physics, 2018, 149, 134110.	1.2	12
26	Atomic-batched tensor decomposed two-electron repulsion integrals. Journal of Chemical Physics, 2017, 146, 134112.	1.2	9
27	Efficient algorithms for solving the non-linear vibrational coupled-cluster equations using full and decomposed tensors. Journal of Chemical Physics, 2017, 146, 134110.	1.2	12
28	Accuracy of Frequencies Obtained with the Aid of Explicitly Correlated Wave Function Based Methods. Journal of Chemical Theory and Computation, 2017, 13, 3602-3613.	2.3	6
29	Density matrices and iterative natural modals in vibrational structure theory. Molecular Physics, 2017, 115, 228-240.	0.8	5
30	FALCON: A method for flexible adaptation of local coordinates of nuclei. Journal of Chemical Physics, 2016, 144, 074108.	1.2	32
31	Linear-scaling generation of potential energy surfaces using a double incremental expansion. Journal of Chemical Physics, 2016, 145, .	1.2	43
32	Calculating vibrational spectra without determining excited eigenstates: Solving the complex linear equations of damped response theory for vibrational configuration interaction and vibrational coupled cluster states. Journal of Chemical Physics, 2015, 143, 134108.	1.2	12
33	Tensor decomposition techniques in the solution of vibrational coupled cluster response theory eigenvalue equations. Journal of Chemical Physics, 2015, 142, 024105.	1.2	17
34	Polarizable Embedded RI-CC2 Method for Two-Photon Absorption Calculations. Journal of Chemical Theory and Computation, 2015, 11, 3669-3678.	2.3	12
35	Experimental and computational study of solvent effects on one- and two-photon absorption spectra of chlorinated harmines. Physical Chemistry Chemical Physics, 2015, 17, 12090-12099.	1.3	20
36	Automatic determination of important modeâ€“mode correlations in many-mode vibrational wave functions. Journal of Chemical Physics, 2015, 142, 144115.	1.2	29

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37	Hybrid Optimized and Localized Vibrational Coordinates. Journal of Physical Chemistry A, 2015, 119, 11007-11021.	1.1	37
38	Lanczos-driven coupledâ€“cluster damped linear response theory for molecules in polarizable environments. Journal of Chemical Physics, 2014, 141, 244107.	1.2	19
39	Optimized coordinates in vibrational coupled cluster calculations. Journal of Chemical Physics, 2014, 140, .	1.2	56
40	Identifying the Hamiltonian structure in linear response theory. Journal of Chemical Physics, 2014, 140, 224103.	1.2	10
41	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	6.2	1,166
42	Coupled cluster calculations of mean excitation energies of the noble gas atoms He, Ne and Ar and of the H2molecule. Molecular Physics, 2014, 112, 751-761.	0.8	12
43	Effect of chromophore encapsulation on linear and nonlinear optical properties: the case of â€œminiSOGâ€, a protein-encased flavin. Physical Chemistry Chemical Physics, 2014, 16, 9950.	1.3	23
44	A simple state-average procedure determining optimal coordinates for anharmonic vibrational calculations. Chemical Physics Letters, 2014, 610-611, 288-297.	1.2	29
45	Ab initio potential energy and dipole moment surfaces of the Fâ¯(H2O) complex. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 119, 59-62.	2.0	20
46	Failures of TDDFT in describing the lowest intramolecular charge-transfer excitation in para-nitroaniline. Molecular Physics, 2013, 111, 1235-1248.	0.8	79
47	Hydrogenâ€Bond Cooperative Effects in Small Cyclic Water Clusters as Revealed by the Interacting Quantum Atoms Approach. Chemistry - A European Journal, 2013, 19, 14304-14315.	1.7	80
48	Photoionization cross section by Stieltjes imaging applied to coupled cluster Lanczos pseudo-spectra. Journal of Chemical Physics, 2013, 139, 094103.	1.2	33
49	Computational screening of one- and two-photon spectrally tuned channelrhodopsin mutants. Physical Chemistry Chemical Physics, 2013, 15, 7567.	1.3	31
50	Tensor Decomposition and Vibrational Coupled Cluster Theory. Journal of Physical Chemistry A, 2013, 117, 7267-7279.	1.1	24
51	A band Lanczos approach for calculation of vibrational coupled cluster response functions: simultaneous calculation of IR and Raman anharmonic spectra for the complex of pyridine and a silver cation. Physical Chemistry Chemical Physics, 2013, 15, 10035.	1.3	15
52	Carbon X-ray absorption spectra of fluoroethenes and acetone: A study at the coupled cluster, density functional, and static-exchange levels of theory. Journal of Chemical Physics, 2013, 138, 124311.	1.2	53
53	Communication: A reduced-space algorithm for the solution of the complex linear response equations used in coupled cluster damped response theory. Journal of Chemical Physics, 2013, 139, 211102.	1.2	45
54	Vibrational absorption spectra from vibrational coupled cluster damped linear response functions calculated using an asymmetric Lanczos algorithm. Journal of Chemical Physics, 2012, 136, 124101.	1.2	26

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55	Approximate inclusion of four-mode couplings in vibrational coupled-cluster theory. Journal of Chemical Physics, 2012, 136, 204118.	1.2	9
56	Selected new developments in vibrational structure theory: potential construction and vibrational wave function calculations. Physical Chemistry Chemical Physics, 2012, 14, 6672.	1.3	121
57	Asymmetric-Lanczos-Chain-Driven Implementation of Electronic Resonance Convergent Coupled-Cluster Linear Response Theory. Journal of Chemical Theory and Computation, 2012, 8, 1616-1628.	2.3	98
58	PERIâ€“CC2: A Polarizable Embedded RI-CC2 Method. Journal of Chemical Theory and Computation, 2012, 8, 3274-3283.	2.3	75
59	Coupled-cluster response theory for near-edge x-ray-absorption fine structure of atoms and molecules. Physical Review A, 2012, 85, .	1.0	137
60	Performance of popular XCâ€functionals for the description of excitation energies in GFPâ€like chromophore models. International Journal of Quantum Chemistry, 2012, 112, 789-800.	1.0	51
61	Excited state coupled cluster methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 566-584.	6.2	165
62	Unraveling the similarity of the photoabsorption of deprotonated p-coumaric acid in the gas phase and within the photoactive yellow protein. Physical Chemistry Chemical Physics, 2011, 13, 1585-1589.	1.3	39
63	Scrutinizing the effects of polarization in QM/MM excited state calculations. Physical Chemistry Chemical Physics, 2011, 13, 18551.	1.3	94
64	Solvation Effects on Electronic Transitions: Exploring the Performance of Advanced Solvent Potentials in Polarizable Embedding Calculations. Journal of Chemical Theory and Computation, 2011, 7, 2209-2217.	2.3	75
65	Vibrational spectroscopy of hydrogen-bonded systems: Six-dimensional simulation of the IR spectrum of Fâ^'(H2O) complex. Chemical Physics Letters, 2011, 510, 36-41.	1.2	10
66	The polarizable embedding coupled cluster method. Journal of Chemical Physics, 2011, 134, 104108.	1.2	117
67	Accurate multimode vibrational calculations using a B-spline basis: theory, tests and application to dioxirane and diazirinone. Molecular Physics, 2011, 109, 673-685.	0.8	33
68	Vibrational coupled cluster response theory: A general implementation. Journal of Chemical Physics, 2011, 134, 054119.	1.2	52
69	Computation of expectation values from vibrational coupled-cluster at the two-mode coupling level. Journal of Chemical Physics, 2011, 134, 154101.	1.2	9
70	Vibrational contributions to cubic response functions from vibrational configuration interaction response theory. Journal of Chemical Physics, 2011, 135, 154107.	1.2	10
71	Spectroscopic Implications of the Electron Donorâ€“Acceptor Effect in the Photoactive Yellow Protein Chromophore. Chemistry - A European Journal, 2010, 16, 11977-11984.	1.7	20
72	Vibrational absorption spectra calculated from vibrational configuration interaction response theory using the Lanczos method. Journal of Chemical Physics, 2010, 132, 164105.	1.2	26

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73	A Lanczos-chain driven approach for calculating damped vibrational configuration interaction response functions. Journal of Chemical Physics, 2010, 133, 114102.	1.2	15
74	Using Electronic Energy Derivative Information in Automated Potential Energy Surface Construction for Vibrational Calculations. Journal of Chemical Theory and Computation, 2010, 6, 3162-3175.	2.3	39
75	Approximate Inclusion of Triple Excitations in Combined Coupled Cluster/Molecular Mechanics: Calculations of Electronic Excitation Energies in Solution for Acrolein, Water, Formamide, and N-Methylacetamide. Journal of Chemical Theory and Computation, 2010, 6, 839-850.	2.3	21
76	New Formulation and Implementation of Vibrational Self-Consistent Field Theory. Journal of Chemical Theory and Computation, 2010, 6, 235-248.	2.3	69
77	Vibrational Coupled Cluster Theory. Challenges and Advances in Computational Chemistry and Physics, 2010, , 491-512.	0.6	5
78	Vibrational coupled cluster theory with full two-mode and approximate three-mode couplings: The VCC[2pt3] model. Journal of Chemical Physics, 2009, 131, 034115.	1.2	29
79	A hierarchy of potential energy surfaces constructed from energies and energy derivatives calculated on grids. Journal of Chemical Physics, 2009, 130, 134104.	1.2	30
80	Automated calculation of anharmonic vibrational contributions to first hyperpolarizabilities: Quadratic response functions from vibrational configuration interaction wave functions. Journal of Chemical Physics, 2009, 131, 154101.	1.2	29
81	An adaptive density-guided approach for the generation of potential energy surfaces of polyatomic molecules. Theoretical Chemistry Accounts, 2009, 123, 413-429.	0.5	73
82	The vibrational auto-adjusting perturbation theory. Theoretical Chemistry Accounts, 2009, 123, 41-49.	0.5	8
83	Vibrational effects in the parity-violating contributions to the isotropic nuclear magnetic resonance chemical shift. Chemical Physics Letters, 2009, 470, 166-171.	1.2	11
84	Linear response coupled cluster study of the benzene excimer. Chemical Physics Letters, 2009, 482, 44-49.	1.2	28
85	On the coupling strength in potential energy surfaces for vibrational calculations. Chemical Physics Letters, 2009, 483, 138-142.	1.2	45
86	Gas Phase Absorption Studies of Photoactive Yellow Protein Chromophore Derivatives. Journal of Physical Chemistry A, 2009, 113, 9442-9449.	1.1	56
87	Automatic derivation and evaluation of vibrational coupled cluster theory equations. Journal of Chemical Physics, 2009, 131, 234109.	1.2	66
88	Photoabsorption studies of neutral green fluorescent protein model chromophores in vacuo. Physical Chemistry Chemical Physics, 2009, 11, 9996.	1.3	41
89	Potential Energy Surfaces for Vibrational Structure Calculations from a Multiresolution Adaptive Density-Guided Approach: Implementation and Test Calculations. Journal of Physical Chemistry A, 2009, 113, 8712-8723.	1.1	34
90	Determination of rate constants for the uptake process involving SO2 and an aerosol particle. A quantum mechanics/molecular mechanics and quantum statistical investigation. Chemical Physics, 2008, 348, 21-30.	0.9	7

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91	Vibrational Contributions to Indirect Spinâ^'Spin Coupling Constants Calculated via Variational Anharmonic Approaches. Journal of Physical Chemistry A, 2008, 112, 8436-8445.	1.1	17
92	Effects of conjugation length and resonance enhancement on two-photon absorption in phenyleneâ€"vinylene oligomers. Physical Chemistry Chemical Physics, 2008, 10, 1177-1191.	1.3	43
93	A virtual vibrational self-consistent-field method for efficient calculation of molecular vibrational partition functions and thermal effects on molecular properties. Journal of Chemical Physics, 2008, 128, 174106.	1.2	21
94	Towards fast computations of correlated vibrational wave functions: Vibrational coupled cluster response excitation energies at the two-mode coupling level. Journal of Chemical Physics, 2008, 128, 154113.	1.2	42
95	On the performance of quantum chemical methods to predict solvatochromic effects: The case of acrolein in aqueous solution. Journal of Chemical Physics, 2008, 128, 194503.	1.2	76
96	Vibrational and thermal effects on the dipole polarizability of methane and carbon tetrachloride from vibrational structure calculations. Journal of Chemical Physics, 2007, 127, 154315.	1.2	18
97	Density functional self-consistent quantum mechanics/molecular mechanics theory for linear and nonlinear molecular properties: Applications to solvated water and formaldehyde. Journal of Chemical Physics, 2007, 126, 154112.	1.2	144
98	Vibrational excitation energies from vibrational coupled cluster response theory. Journal of Chemical Physics, 2007, 126, 204101.	1.2	84
99	Variational calculation of static and dynamic vibrational nonlinear optical properties. Journal of Chemical Physics, 2007, 127, 084118.	1.2	29
100	Automatic generation of potential energy and property surfaces of polyatomic molecules in normal coordinates. Journal of Chemical Physics, 2007, 127, 204106.	1.2	54
101	Treatment of Vibronic Interactions Using Variational Methods for Nuclear Motion. AIP Conference Proceedings, 2007, , .	0.3	0
102	Nuclear magnetic shielding constants of liquid water: Insights from hybrid quantum mechanics/molecular mechanics models. Journal of Chemical Physics, 2007, 126, 034510.	1.2	59
103	General biorthogonal projected bases as applied to second-order MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2007, 127, 074106.	1.2	30
104	One- and Two-Photon Photosensitized Singlet Oxygen Production:Â Characterization of Aromatic Ketones as Sensitizer Standards. Journal of Physical Chemistry A, 2007, 111, 5756-5767.	1.1	61
105	Vibrational structure theory: new vibrational wave function methods for calculation of anharmonic vibrational energies and vibrational contributions to molecular properties. Physical Chemistry Chemical Physics, 2007, 9, 2942.	1.3	232
106	Two-Photon Absorption in Tetraphenylporphycenes:Â Are Porphycenes Better Candidates than Porphyrins for Providing Optimal Optical Properties for Two-Photon Photodynamic Therapy?. Journal of the American Chemical Society, 2007, 129, 5188-5199.	6.6	189
107	Calculation of Vibrational Infrared Intensities and Raman Activities Using Explicit Anharmonic Wave Functions. Journal of Physical Chemistry A, 2007, 111, 11205-11213.	1.1	43
108	Solvent Effects on NMR Isotropic Shielding Constants. A Comparison between Explicit Polarizable Discrete and Continuum Approaches. Journal of Physical Chemistry A, 2007, 111, 4199-4210.	1.1	74

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109	Gauge-origin independent magnetizabilities from hybrid quantum mechanics/molecular mechanics models: Theory and applications to liquid water. Chemical Physics Letters, 2007, 442, 322-328.	1.2	3
110	Coupled-cluster theory in a projected atomic orbital basis. Journal of Chemical Physics, 2006, 124, 084103.	1.2	44
111	Uptake of Phenol on Aerosol Particlesâ€. Journal of Physical Chemistry A, 2006, 110, 660-670.	1.1	18
112	THE (HYPER)POLARIZABILITIES OF LIQUID WATER MODELLED USING COUPLED CLUSTER/MOLECULAR MECHANICS RESPONSE THEORY METHODS. , 2006, , 215-281.		0
113	The electronic spectrum of the micro-solvated alanine zwitterion calculated using the combined coupled cluster/molecular mechanics method. Chemical Physics Letters, 2006, 429, 430-435.	1.2	19
114	Overview of Theoretical and Computational Methods Applied to the Oxygenâ€“Organic Molecule Photosystem. Photochemistry and Photobiology, 2006, 82, 1136.	1.3	104
115	Coupled Cluster Theory with Emphasis on Selected New Developments. Theoretical Chemistry Accounts, 2006, 116, 106-123.	0.5	59
116	Automatic generation of force fields and property surfaces for use in variational vibrational calculations of anharmonic vibrational energies and zero-point vibrational averaged properties. Journal of Chemical Physics, 2006, 125, 124108.	1.2	72
117	A variational approach for calculating Franck-Condon factors including mode-mode anharmonic coupling. Journal of Chemical Physics, 2006, 125, 154114.	1.2	36
118	Benchmarking two-photon absorption with CC3 quadratic response theory, and comparison with density-functional response theory. Journal of Chemical Physics, 2006, 124, 054322.	1.2	137
119	Linear response functions for a vibrational configuration interaction state. Journal of Chemical Physics, 2006, 125, 214309.	1.2	51
120	Statistical mechanically averaged molecular properties of liquid water calculated using the combined coupled cluster/molecular dynamics method. Journal of Chemical Physics, 2006, 124, 124503.	1.2	55
121	Accurate Nonlinear Optical Properties for Small Molecules. Challenges and Advances in Computational Chemistry and Physics, 2006, , 51-99.	0.6	23
122	Two-photon absorption cross sections: An investigation of solvent effects. Theoretical studies on formaldehyde and water. Journal of Chemical Physics, 2006, 125, 184501.	1.2	35
123	Beyond vibrational self-consistent-field methods: Benchmark calculations for the fundamental vibrations of ethylene. International Journal of Quantum Chemistry, 2005, 104, 667-680.	1.0	62
124	â€‡Response theory for vibrational wave functions. Journal of Chemical Physics, 2005, 122, 194105.	1.2	60
125	Theoretical Study of the Electronic Gas-Phase Spectrum of Glycine, Alanine, and Related Amines and Carboxylic Acids. Journal of Physical Chemistry A, 2005, 109, 1430-1440.	1.1	51
126	Coupled Cluster Calculation of the n â†' Ï€* Electronic Transition of Acetone in Aqueous Solution. Journal of Physical Chemistry A, 2005, 109, 8001-8010.	1.1	107

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127	Solvent effects on the nâ†'Ï€[sup â^—] electronic transition in formaldehyde: A combined coupled cluster/molecular dynamics study. Journal of Chemical Physics, 2004, 121, 8435.	1.2	75
128	Vibrational coupled cluster theory. Journal of Chemical Physics, 2004, 120, 2149-2159.	1.2	289
129	A coupled cluster study of the oriented circular dichroism of the nâ†'Ï€â^— electronic transition in cyclopropanone and natural optical active related structures. Chemical Physics Letters, 2004, 391, 259-266.	1.2	18
130	Second harmonic generation second hyperpolarizability of water calculated using the combined coupled cluster dielectric continuum or different molecular mechanics methods. Journal of Chemical Physics, 2004, 120, 3787-3798.	1.2	67
131	A second quantization formulation of multimode dynamics. Journal of Chemical Physics, 2004, 120, 2140-2148.	1.2	127
132	Fast Photodynamics of Aqueous Formic Acid. Journal of Physical Chemistry A, 2004, 108, 7483-7489.	1.1	12
133	Linear Response Properties of Liquid Water Calculated Using CC2 and CCSD within Different Molecular Mechanics Methodsâ€. Journal of Physical Chemistry A, 2004, 108, 8646-8658.	1.1	52
134	Thenâ†' Ï€* Electronic Transition in Microsolvated Formaldehyde. A Coupled Cluster and Combined Coupled Cluster/Molecular Mechanics Studyâ€. Journal of Physical Chemistry A, 2004, 108, 8624-8632.	1.1	44
135	Solvent Effects on Rotatory Strength Tensors. 1. Theory and Application of the Combined Coupled Cluster/Dielectric Continuum Model. Journal of Physical Chemistry A, 2004, 108, 3632-3641.	1.1	42
136	Molecular electric properties of liquid water calculated using the combined coupled cluster/molecular mechanics method. Computational and Theoretical Chemistry, 2003, 632, 207-225.	1.5	14
137	Coupled Cluster/Molecular Mechanics Method:â€‰ Implementation and Application to Liquid Water. Journal of Physical Chemistry A, 2003, 107, 2578-2588.	1.1	70
138	A CC2 dielectric continuum model and a CC2 molecular mechanics model. Molecular Physics, 2003, 101, 2055-2071.	0.8	37
139	MÃ¸llerâ€“Plesset perturbation theory for vibrational wave functions. Journal of Chemical Physics, 2003, 119, 5773-5781.	1.2	186
140	Linear response functions for coupled cluster/molecular mechanics including polarization interactions. Journal of Chemical Physics, 2003, 118, 1620-1633.	1.2	117
141	Nonlinear optical response properties of molecules in condensed phases using the coupled cluster/dielectric continuum or molecular mechanics methods. Journal of Chemical Physics, 2003, 119, 10519-10535.	1.2	55
142	On the electric field gradient induced birefringence and electric quadrupole moment of CO, N[sub 2]O, and OCS. Journal of Chemical Physics, 2003, 118, 7329.	1.2	37
143	Vibronic transitions from coupled-cluster response theory: Theory and application to HSiF and H[sub 2]O. Journal of Chemical Physics, 2002, 116, 8334.	1.2	8
144	Implementation of electronic ground states and singlet and triplet excitation energies in coupled cluster theory with approximate triples corrections. Journal of Chemical Physics, 2002, 116, 5963-5970.	1.2	32

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145	The QM/MM approach for wavefunctions, energies and response functions within self-consistent field and coupled cluster theories. Molecular Physics, 2002, 100, 1813-1828.	0.8	122
146	Radiative singletâ€“triplet transition properties from coupled-cluster response theory: The importance of the S0â†'T1 transition for the photodissociation of water at 193 nm. Journal of Chemical Physics, 2002, 116, 6674-6686.	1.2	7
147	A coupled cluster response study of the electric dipole polarizability, first and second hyperpolarizabilities of HCl. Physical Chemistry Chemical Physics, 2002, 4, 2884-2890.	1.3	15
148	Electric field gradients of water: A systematic investigation of basis set, electron correlation, and rovibrational effects. Journal of Chemical Physics, 2002, 116, 1424-1434.	1.2	20
149	Dipole and quadrupole moments of liquid water calculated within the coupled cluster/molecular mechanics method. Chemical Physics Letters, 2002, 364, 379-386.	1.2	47
150	Ab initio modeling of excited state absorption of polyenes. Physical Chemistry Chemical Physics, 2001, 3, 2567-2575.	1.3	35
151	Electronic excitation energies of pyrimidine studied using coupled cluster response theory. Physical Chemistry Chemical Physics, 2001, 3, 730-740.	1.3	25
152	Equilibrium geometries of cyclic SiC3 isomers. Journal of Chemical Physics, 2001, 114, 2993-2995.	1.2	50
153	Triple excitation effects in coupled cluster calculations of Verdet constants. Chemical Physics Letters, 2000, 330, 463-470.	1.2	20
154	Spin-orbit coupling constants from coupled-cluster response theory. Physical Chemistry Chemical Physics, 2000, 2, 965-971.	1.3	97
155	Coupled cluster investigation of Sternheimer shieldings and electric field gradient polarizabilities. Journal of Chemical Physics, 2000, 113, 1688-1697.	1.2	7
156	Divergence in MÃ¸llerâ€“Plesset theory: A simple explanation based on a two-state model. Journal of Chemical Physics, 2000, 112, 9736-9748.	1.2	79
157	Atomic integral driven second order polarization propagator calculations of the excitation spectra of naphthalene and anthracene. Journal of Chemical Physics, 2000, 112, 4173-4185.	1.2	131
158	A theoretical study of the electronic spectrum of water. Journal of Chemical Physics, 2000, 113, 8101-8112.	1.2	68
159	Full configuration interaction benchmarking of coupled-cluster models for the lowest singlet energy surfaces of N2. Journal of Chemical Physics, 2000, 113, 6677-6686.	1.2	109
160	Theoretical calculations of excited state absorption. Physical Chemistry Chemical Physics, 2000, 2, 5357-5363.	1.3	37
161	Two-photon dissociation and ionization of liquid water studied by femtosecond transient absorption spectroscopy. Journal of Chemical Physics, 1999, 110, 3453-3462.	1.2	177
162	Coupled cluster response theory for solvated molecules in equilibrium and nonequilibrium solvation. Journal of Chemical Physics, 1999, 110, 8348-8360.	1.2	99

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163	A coupled-cluster solvent reaction field method. Journal of Chemical Physics, 1999, 110, 1365-1375.	1.2	93
164	The electronic spectrum of pyrrole. Journal of Chemical Physics, 1999, 111, 525-537.	1.2	117
165	First-order nonadiabatic coupling matrix elements using coupled cluster methods. I. Theory. Journal of Chemical Physics, 1999, 110, 711-723.	1.2	30
166	Ground and excited state polarizabilities and dipole transition properties of benzene from coupled cluster response theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1999, 55, 509-524.	2.0	37
167	Frequency-dependent polarizabilities and first hyperpolarizabilities of CO and H2O from coupled cluster calculations. Chemical Physics Letters, 1999, 305, 147-155.	1.2	219
168	Polarizabilities and first hyperpolarizabilities of HF, Ne, and BH from full configuration interaction and coupled cluster calculations. Journal of Chemical Physics, 1999, 111, 1917-1925.	1.2	89
169	Frequency-dependent second hyperpolarizabilities using coupled cluster cubic response theory. Chemical Physics Letters, 1998, 282, 139-146.	1.2	108
170	A second-order doubles correction to excitation energies in the random-phase approximation. Chemical Physics Letters, 1998, 284, 47-55.	1.2	39
171	The effect of triple excitations in coupled cluster calculations of frequency-dependent polarizabilities. Chemical Physics Letters, 1998, 292, 437-446.	1.2	61
172	Triple excitation effects in coupled-cluster calculations of frequency-dependent hyperpolarizabilities. Chemical Physics Letters, 1998, 296, 117-124.	1.2	56
173	Polarizabilities of CO, N2, HF, Ne, BH, and CH+ from ab initio calculations: Systematic studies of electron correlation, basis set errors, and vibrational contributions. Journal of Chemical Physics, 1998, 109, 4745-4757.	1.2	127
174	Response functions from Fourier component variational perturbation theory applied to a time-averaged quasienergy. International Journal of Quantum Chemistry, 1998, 68, 1-52.	1.0	497
175	The Electronic Spectrum of Furan. Journal of the American Chemical Society, 1998, 120, 3423-3430.	6.6	74
176	A coupled cluster study of the 1â€‰1A1g and 1â€‰1B2u states of benzene. Journal of Chemical Physics, 1998, 108, 3987-4001.	1.2	72
177	Multiphoton transition moments and absorption cross sections in coupled cluster response theory employing variational transition moment functionals. Journal of Chemical Physics, 1998, 108, 8331-8354.	1.2	90
178	Integral-direct coupled cluster calculations of frequency-dependent polarizabilities, transition probabilities and excited-state properties. Journal of Chemical Physics, 1998, 108, 2801-2816.	1.2	191
179	The benzeneâ€“argon complex: A ground and excited state ab initio study. Journal of Chemical Physics, 1998, 108, 2784-2790.	1.2	144
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