Ove Christiansen

List of Publications by Year in Descending Order

204 papers	13,733 citations	63 h-index	111 g-index
207 ext. papers	14,413 ext. citations	3.6 avg, IF	6.55 L-index

#	Paper	IF	Citations
204	Vibrational Coupled Cluster Theory **2022**, 41-79		
203	Calculating vibrational excitation energies using tensor-decomposed vibrational coupled-cluster response theory. *Journal of Chemical Physics*, **2021**, 154, 054113	3.9	2
202	Bypassing the computational bottleneck of quantum-embedding theories for strong electron correlations with machine learning. *Physical Review Research*, **2021**, 3,	3.9	1
201	Time-dependent vibrational coupled cluster with variationally optimized time-dependent basis sets. *Journal of Chemical Physics*, **2020**, 153, 174108	3.9	5
200	Vibrational Coupled Cluster Computations in Polyspherical Coordinates with the Exact Analytical Kinetic Energy Operator. *Journal of Chemical Theory and Computation*, **2020**, 16, 4505-4520	6.4	2
199	MR-MCTDH[]: Flexible Configuration Spaces and Nonadiabatic Dynamics within the MCTDH[] Framework. *Journal of Chemical Theory and Computation*, **2020**, 16, 4087-4097	6.4	5
198	Toward Accurate Theoretical Vibrational Spectra: A Case Study for Maleimide. *Journal of Physical Chemistry A*, **2020**, 124, 2616-2627	2.8	5
197	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	3.9	9
196	Adaptive density-guided approach to double incremental potential energy surface construction. *Journal of Chemical Physics*, **2020**, 152, 194105	3.9	2
195	Vibrationally resolved coupled-cluster x-ray absorption spectra from vibrational configuration interaction anharmonic calculations. *Journal of Chemical Physics*, **2020**, 153, 234111	3.9	3
194	A general implementation of time-dependent vibrational coupled-cluster theory. *Journal of Chemical Physics*, **2020**, 153, 234109	3.9	2
193	Extended vibrational coupled cluster: Stationary states and dynamics. *Journal of Chemical Physics*, **2020**, 153, 044133	3.9	6
192	A Gaussian process regression adaptive density guided approach for potential energy surface construction.. *Journal of Chemical Physics*, **2020**, 153, 064105	3.9	9
191	Time-dependent vibrational coupled cluster theory: Theory and implementation at the two-mode coupling level. *Journal of Chemical Physics*, **2019**, 151, 154116	3.9	10
190	Approximate high mode coupling potentials using Gaussian process regression and adaptive density guided sampling. *Journal of Chemical Physics*, **2019**, 150, 131102	3.9	28
189	Vibrationally resolved emission spectra of luminescent conjugated oligothiophenes from anharmonic calculations. *Physical Chemistry Chemical Physics*, **2019**, 21, 17410-17422	3.6	11
188	Machine learning for potential energy surfaces: An extensive database and assessment of methods. *Journal of Chemical Physics*, **2019**, 150, 244113	3.9	29

187	Assessment of the overlap metric in the context of RI-MP2 and atomic batched tensor decomposed MP2. *Chemical Physics Letters*, **2018**, 701, 7-14	2.5	2
186	Employing general fit-bases for construction of potential energy surfaces with an adaptive density-guided approach. *Journal of Chemical Physics*, **2018**, 148, 064113	3.9	17
185	Tensor-decomposed vibrational coupled-cluster theory: Enabling large-scale, highly accurate vibrational-structure calculations. *Journal of Chemical Physics*, **2018**, 148, 024103	3.9	15
184	Anharmonic vibrational spectra from double incremental potential energy and dipole surfaces. *Physical Chemistry Chemical Physics*, **2018**, 20, 3445-3456	3.6	15
183	Gaussian process regression to accelerate geometry optimizations relying on numerical differentiation. *Journal of Chemical Physics*, **2018**, 148, 241704	3.9	37
182	Describing Molecules in Motion by Quantum Many-Body Methods **2018**, 199-221		
181	Exponential parameterization of wave functions for quantum dynamics: Time-dependent Hartree in second quantization. *Journal of Chemical Physics*, **2018**, 149, 134110	3.9	9
180	Atomic-batched tensor decomposed two-electron repulsion integrals. *Journal of Chemical Physics*, **2017**, 146, 134112	3.9	8
179	Efficient algorithms for solving the non-linear vibrational coupled-cluster equations using full and decomposed tensors. *Journal of Chemical Physics*, **2017**, 146, 134110	3.9	10
178	Accuracy of Frequencies Obtained with the Aid of Explicitly Correlated Wave Function Based Methods. *Journal of Chemical Theory and Computation*, **2017**, 13, 3602-3613	6.4	5
177	Density matrices and iterative natural modals in vibrational structure theory. *Molecular Physics*, **2017**, 115, 228-240	1.7	3
176	FALCON: A method for flexible adaptation of local coordinates of nuclei. *Journal of Chemical Physics*, **2016**, 144, 074108	3.9	25
175	Linear-scaling generation of potential energy surfaces using a double incremental expansion. *Journal of Chemical Physics*, **2016**, 145, 064105	3.9	32
174	Polarizable Embedded RI-CC2 Method for Two-Photon Absorption Calculations. *Journal of Chemical Theory and Computation*, **2015**, 11, 3669-78	6.4	11
173	Experimental and computational study of solvent effects on one- and two-photon absorption spectra of chlorinated harmines. *Physical Chemistry Chemical Physics*, **2015**, 17, 12090-9	3.6	17
172	Automatic determination of important mode-mode correlations in many-mode vibrational wave functions. *Journal of Chemical Physics*, **2015**, 142, 144115	3.9	22
171	Hybrid Optimized and Localized Vibrational Coordinates. *Journal of Physical Chemistry A*, **2015**, 119, 11007-21	2.8	29
170	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	3.9	10

169	Tensor decomposition techniques in the solution of vibrational coupled cluster response theory eigenvalue equations. *Journal of Chemical Physics*, **2015**, 142, 024105	3.9	14
168	The Dalton quantum chemistry program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 269-284	7.9	956
167	Coupled cluster calculations of mean excitation energies of the noble gas atoms He, Ne and Ar and of the H2 molecule. *Molecular Physics*, **2014**, 112, 751-761	1.7	11
166	Effect of chromophore encapsulation on linear and nonlinear optical properties: the case of "miniSOG", a protein-encased flavin. *Physical Chemistry Chemical Physics*, **2014**, 16, 9950-9	3.6	19
165	A simple state-average procedure determining optimal coordinates for anharmonic vibrational calculations. *Chemical Physics Letters*, **2014**, 610-611, 288-297	2.5	25
164	Ab initio potential energy and dipole moment surfaces of the F(-)(H2O) complex. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 119, 59-62	4.4	17
163	Lanczos-driven coupled-cluster damped linear response theory for molecules in polarizable environments. *Journal of Chemical Physics*, **2014**, 141, 244107	3.9	19
162	Optimized coordinates in vibrational coupled cluster calculations. *Journal of Chemical Physics*, **2014**, 140, 154102	3.9	47
161	Identifying the Hamiltonian structure in linear response theory. *Journal of Chemical Physics*, **2014**, 140, 224103	3.9	10
160	Failures of TDDFT in describing the lowest intramolecular charge-transfer excitation in para-nitroaniline. *Molecular Physics*, **2013**, 111, 1235-1248	1.7	71
159	Hydrogen-bond cooperative effects in small cyclic water clusters as revealed by the interacting quantum atoms approach. *Chemistry - A European Journal*, **2013**, 19, 14304-15	4.8	71
158	Photoionization cross section by Stieltjes imaging applied to coupled cluster Lanczos pseudo-spectra. *Journal of Chemical Physics*, **2013**, 139, 094103	3.9	31
157	Computational screening of one- and two-photon spectrally tuned channelrhodopsin mutants. *Physical Chemistry Chemical Physics*, **2013**, 15, 7567-76	3.6	25
156	Tensor decomposition and vibrational coupled cluster theory. *Journal of Physical Chemistry A*, **2013**, 117, 7267-79	2.8	18
155	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, 10035-48	3.6	11
154	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	3.9	44
153	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	3.9	39
152	Selected new developments in vibrational structure theory: potential construction and vibrational wave function calculations. *Physical Chemistry Chemical Physics*, **2012**, 14, 6672-87	3.6	101

151	Asymmetric-Lanczos-Chain-Driven Implementation of Electronic Resonance Convergent Coupled-Cluster Linear Response Theory. *Journal of Chemical Theory and Computation*, **2012**, 8, 1616-28	6.4	87
150	PERI-CC2: A Polarizable Embedded RI-CC2 Method. *Journal of Chemical Theory and Computation*, **2012**, 8, 3274-83	6.4	66
149	Coupled-cluster response theory for near-edge x-ray-absorption fine structure of atoms and molecules. *Physical Review A*, **2012**, 85,	2.6	117
148	Performance of popular XC-functionals for the description of excitation energies in GFP-like chromophore models. *International Journal of Quantum Chemistry*, **2012**, 112, 789-800	2.1	45
147	Excited state coupled cluster methods. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 566-584	7.9	132
146	Vibrational absorption spectra from vibrational coupled cluster damped linear response functions calculated using an asymmetric Lanczos algorithm. *Journal of Chemical Physics*, **2012**, 136, 124101	3.9	22
145	Approximate inclusion of four-mode couplings in vibrational coupled-cluster theory. *Journal of Chemical Physics*, **2012**, 136, 204118	3.9	8
144	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, 1585-9	3.6	37
143	Scrutinizing the effects of polarization in QM/MM excited state calculations. *Physical Chemistry Chemical Physics*, **2011**, 13, 18551-60	3.6	84
142	Solvation Effects on Electronic Transitions: Exploring the Performance of Advanced Solvent Potentials in Polarizable Embedding Calculations. *Journal of Chemical Theory and Computation*, **2011**, 7, 2209-17	6.4	70
141	Vibrational spectroscopy of hydrogen-bonded systems: Six-dimensional simulation of the IR spectrum of F(H2O) complex. *Chemical Physics Letters*, **2011**, 510, 36-41	2.5	10
140	The polarizable embedding coupled cluster method. *Journal of Chemical Physics*, **2011**, 134, 104108	3.9	106
139	Accurate multimode vibrational calculations using a B-spline basis: theory, tests and application to dioxirane and diazirinone. *Molecular Physics*, **2011**, 109, 673-685	1.7	27
138	Vibrational coupled cluster response theory: a general implementation. *Journal of Chemical Physics*, **2011**, 134, 054119	3.9	45
137	Computation of expectation values from vibrational coupled-cluster at the two-mode coupling level. *Journal of Chemical Physics*, **2011**, 134, 154101	3.9	7
136	Vibrational contributions to cubic response functions from vibrational configuration interaction response theory. *Journal of Chemical Physics*, **2011**, 135, 154107	3.9	10
135	Vibrational absorption spectra calculated from vibrational configuration interaction response theory using the Lanczos method. *Journal of Chemical Physics*, **2010**, 132, 164105	3.9	25
134	A Lanczos-chain driven approach for calculating damped vibrational configuration interaction response functions. *Journal of Chemical Physics*, **2010**, 133, 114102	3.9	13

133	Using Electronic Energy Derivative Information in Automated Potential Energy Surface Construction for Vibrational Calculations. *Journal of Chemical Theory and Computation*, **2010**, 6, 3162-75	6.4	34
132	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, 839-50	6.4	19
131	New Formulation and Implementation of Vibrational Self-Consistent Field Theory. *Journal of Chemical Theory and Computation*, **2010**, 6, 235-48	6.4	59
130	Spectroscopic implications of the electron donor-acceptor effect in the photoactive yellow protein chromophore. *Chemistry - A European Journal*, **2010**, 16, 11977-84	4.8	20
129	Vibrational Coupled Cluster Theory. *Challenges and Advances in Computational Chemistry and Physics*, **2010**, 491-512	0.7	5
128	Vibrational coupled cluster theory with full two-mode and approximate three-mode couplings: the VCC[2pt3] model. *Journal of Chemical Physics*, **2009**, 131, 034115	3.9	27
127	A hierarchy of potential energy surfaces constructed from energies and energy derivatives calculated on grids. *Journal of Chemical Physics*, **2009**, 130, 134104	3.9	30
126	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	3.9	28
125	An adaptive density-guided approach for the generation of potential energy surfaces of polyatomic molecules. *Theoretical Chemistry Accounts*, **2009**, 123, 413-429	1.9	63
124	The vibrational auto-adjusting perturbation theory. *Theoretical Chemistry Accounts*, **2009**, 123, 41-49	1.9	8
123	Vibrational effects in the parity-violating contributions to the isotropic nuclear magnetic resonance chemical shift. *Chemical Physics Letters*, **2009**, 470, 166-171	2.5	8
122	Linear response coupled cluster study of the benzene excimer. *Chemical Physics Letters*, **2009**, 482, 44-49	2.5	23
121	On the coupling strength in potential energy surfaces for vibrational calculations. *Chemical Physics Letters*, **2009**, 483, 138-142	2.5	43
120	Gas phase absorption studies of photoactive yellow protein chromophore derivatives. *Journal of Physical Chemistry A*, **2009**, 113, 9442-9	2.8	52
119	Automatic derivation and evaluation of vibrational coupled cluster theory equations. *Journal of Chemical Physics*, **2009**, 131, 234109	3.9	60
118	Photoabsorption studies of neutral green fluorescent protein model chromophores in vacuo. *Physical Chemistry Chemical Physics*, **2009**, 11, 9996-10002	3.6	40
117	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, 8712-23	2.8	27
116	Vibrational contributions to indirect spin-spin coupling constants calculated via variational anharmonic approaches. *Journal of Physical Chemistry A*, **2008**, 112, 8436-45	2.8	17

115	Effects of conjugation length and resonance enhancement on two-photon absorption in phenylene-vinylene oligomers. *Physical Chemistry Chemical Physics*, **2008**, 10, 1177-91	3.6	41
114	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	3.9	18
113	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	3.9	40
112	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	3.9	68
111	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	2.3	7
110	One- and two-photon photosensitized singlet oxygen production: characterization of aromatic ketones as sensitizer standards. *Journal of Physical Chemistry A*, **2007**, 111, 5756-67	2.8	56
109	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, 2942-53	3.6	205
108	Two-photon absorption in tetraphenylporphycenes: are porphycenes better candidates than porphyrins for providing optimal optical properties for two-photon photodynamic therapy?. *Journal of the American Chemical Society*, **2007**, 129, 5188-99	16.4	173
107	Calculation of vibrational infrared intensities and Raman activities using explicit anharmonic wave functions. *Journal of Physical Chemistry A*, **2007**, 111, 11205-13	2.8	36
106	Solvent effects on NMR isotropic shielding constants. a comparison between explicit polarizable discrete and continuum approaches. *Journal of Physical Chemistry A*, **2007**, 111, 4199-210	2.8	73
105	Gauge-origin independent magnetizabilities from hybrid quantum mechanics/molecular mechanics models: Theory and applications to liquid water. *Chemical Physics Letters*, **2007**, 442, 322-328	2.5	3
104	Vibrational and thermal effects on the dipole polarizability of methane and carbon tetrachloride from vibrational structure calculations. *Journal of Chemical Physics*, **2007**, 127, 154315	3.9	17
103	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	3.9	135
102	Vibrational excitation energies from vibrational coupled cluster response theory. *Journal of Chemical Physics*, **2007**, 126, 204101	3.9	77
101	Variational calculation of static and dynamic vibrational nonlinear optical properties. *Journal of Chemical Physics*, **2007**, 127, 084118	3.9	28
100	Automatic generation of potential energy and property surfaces of polyatomic molecules in normal coordinates. *Journal of Chemical Physics*, **2007**, 127, 204106	3.9	51
99	Nuclear magnetic shielding constants of liquid water: insights from hybrid quantum mechanics/molecular mechanics models. *Journal of Chemical Physics*, **2007**, 126, 034510	3.9	57
98	General biorthogonal projected bases as applied to second-order Møller-Plesset perturbation theory. *Journal of Chemical Physics*, **2007**, 127, 074106	3.9	28

97	Coupled Cluster Theory with Emphasis on Selected New Developments. *Theoretical Chemistry Accounts*, **2006**, 116, 106-123	1.9	51
96	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	3.9	69
95	A variational approach for calculating Franck-Condon factors including mode-mode anharmonic coupling. *Journal of Chemical Physics*, **2006**, 125, 154114	3.9	33
94	Benchmarking two-photon absorption with CC3 quadratic response theory, and comparison with density-functional response theory. *Journal of Chemical Physics*, **2006**, 124, 054322	3.9	125
93	Linear response functions for a vibrational configuration interaction state. *Journal of Chemical Physics*, **2006**, 125, 214309	3.9	49
92	Statistical mechanically averaged molecular properties of liquid water calculated using the combined coupled cluster/molecular dynamics method. *Journal of Chemical Physics*, **2006**, 124, 124503	3.9	50
91	Accurate Nonlinear Optical Properties for Small Molecules. *Challenges and Advances in Computational Chemistry and Physics*, **2006**, 51-99	0.7	20
90	Two-photon absorption cross sections: an investigation of solvent effects. Theoretical studies on formaldehyde and water. *Journal of Chemical Physics*, **2006**, 125, 184501	3.9	30
89	Coupled-cluster theory in a projected atomic orbital basis. *Journal of Chemical Physics*, **2006**, 124, 084103	3.9	42
88	Uptake of phenol on aerosol particles. *Journal of Physical Chemistry A*, **2006**, 110, 660-70	2.8	18
87	THE (HYPER)POLARIZABILITIES OF LIQUID WATER MODELLED USING COUPLED CLUSTER/MOLECULAR MECHANICS RESPONSE THEORY METHODS **2006**, 215-281		
86	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	2.5	18
85	Overview of theoretical and computational methods applied to the oxygen-organic molecule photosystem. *Photochemistry and Photobiology*, **2006**, 82, 1136-60	3.6	94
84	Theoretical study of the electronic gas-phase spectrum of glycine, alanine, and related amines and carboxylic acids. *Journal of Physical Chemistry A*, **2005**, 109, 1430-40	2.8	48
83	Coupled cluster calculation of the n --> pi* electronic transition of acetone in aqueous solution. *Journal of Physical Chemistry A*, **2005**, 109, 8001-10	2.8	101
82	Beyond vibrational self-consistent-field methods: Benchmark calculations for the fundamental vibrations of ethylene. *International Journal of Quantum Chemistry*, **2005**, 104, 667-680	2.1	56
81	Response theory for vibrational wave functions. *Journal of Chemical Physics*, **2005**, 122, 194105	3.9	58
80	Solvent effects on the n-->pi* electronic transition in formaldehyde: a combined coupled cluster/molecular dynamics study. *Journal of Chemical Physics*, **2004**, 121, 8435-45	3.9	71

79	Vibrational coupled cluster theory. *Journal of Chemical Physics*, **2004**, 120, 2149-59	3.9	248
78	A coupled cluster study of the oriented circular dichroism of the n->π* electronic transition in cyclopropanone and natural optical active related structures. *Chemical Physics Letters*, **2004**, 391, 259-266	2.5	18
77	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, 3787-98	3.9	64
76	A second quantization formulation of multimode dynamics. *Journal of Chemical Physics*, **2004**, 120, 2140-8	3.9	108
75	Fast Photodynamics of Aqueous Formic Acid. *Journal of Physical Chemistry A*, **2004**, 108, 7483-7489	2.8	11
74	Linear Response Properties of Liquid Water Calculated Using CC2 and CCSD within Different Molecular Mechanics Methods. *Journal of Physical Chemistry A*, **2004**, 108, 8646-8658	2.8	50
73	The n -> π* Electronic Transition in Microsolvated Formaldehyde. A Coupled Cluster and Combined Coupled Cluster/Molecular Mechanics Study. *Journal of Physical Chemistry A*, **2004**, 108, 8624-8632	2.8	43
72	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	2.8	41
71	Molecular electric properties of liquid water calculated using the combined coupled cluster/molecular mechanics method. *Computational and Theoretical Chemistry*, **2003**, 632, 207-225		14
70	Coupled Cluster/Molecular Mechanics Method: Implementation and Application to Liquid Water. *Journal of Physical Chemistry A*, **2003**, 107, 2578-2588	2.8	69
69	A CC2 dielectric continuum model and a CC2 molecular mechanics model. *Molecular Physics*, **2003**, 101, 2055-2071	1.7	36
68	Møller-Plesset perturbation theory for vibrational wave functions. *Journal of Chemical Physics*, **2003**, 119, 5773-5781	3.9	166
67	Linear response functions for coupled cluster/molecular mechanics including polarization interactions. *Journal of Chemical Physics*, **2003**, 118, 1620-1633	3.9	111
66	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	3.9	54
65	On the electric field gradient induced birefringence and electric quadrupole moment of CO, N2O, and OCS. *Journal of Chemical Physics*, **2003**, 118, 7329	3.9	34
64	Dipole and quadrupole moments of liquid water calculated within the coupled cluster/molecular mechanics method. *Chemical Physics Letters*, **2002**, 364, 379-386	2.5	45
63	Vibronic transitions from coupled-cluster response theory: Theory and application to HSiF and H[sub 2]O. *Journal of Chemical Physics*, **2002**, 116, 8334	3.9	8
62	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	3.9	30

61	The QM/MM approach for wavefunctions, energies and response functions within self-consistent field and coupled cluster theories. *Molecular Physics*, **2002**, 100, 1813-1828	1.7	112
60	Radiative singlet–triplet transition properties from coupled-cluster response theory: The importance of the S0->T1 transition for the photodissociation of water at 193 nm. *Journal of Chemical Physics*, **2002**, 116, 6674-6686	3.9	6
59	A coupled cluster response study of the electric dipole polarizability, first and second hyperpolarizabilities of HCl. *Physical Chemistry Chemical Physics*, **2002**, 4, 2884-2890	3.6	14
58	Electric field gradients of water: A systematic investigation of basis set, electron correlation, and rovibrational effects. *Journal of Chemical Physics*, **2002**, 116, 1424-1434	3.9	20
57	Equilibrium geometries of cyclic SiC3 isomers. *Journal of Chemical Physics*, **2001**, 114, 2993-2995	3.9	45
56	Ab initio modeling of excited state absorption of polyenes. *Physical Chemistry Chemical Physics*, **2001**, 3, 2567-2575	3.6	34
55	Electronic excitation energies of pyrimidine studied using coupled cluster response theory. *Physical Chemistry Chemical Physics*, **2001**, 3, 730-740	3.6	24
54	Triple excitation effects in coupled cluster calculations of Verdet constants. *Chemical Physics Letters*, **2000**, 330, 463-470	2.5	19
53	Spin-orbit coupling constants from coupled-cluster response theory. *Physical Chemistry Chemical Physics*, **2000**, 2, 965-971	3.6	83
52	Coupled cluster investigation of Sternheimer shieldings and electric field gradient polarizabilities. *Journal of Chemical Physics*, **2000**, 113, 1688-1697	3.9	6
51	Divergence in Møller–Plesset theory: A simple explanation based on a two-state model. *Journal of Chemical Physics*, **2000**, 112, 9736-9748	3.9	71
50	Atomic integral driven second order polarization propagator calculations of the excitation spectra of naphthalene and anthracene. *Journal of Chemical Physics*, **2000**, 112, 4173-4185	3.9	122
49	A theoretical study of the electronic spectrum of water. *Journal of Chemical Physics*, **2000**, 113, 8101-8112	3.9	65
48	Full configuration interaction benchmarking of coupled-cluster models for the lowest singlet energy surfaces of N2. *Journal of Chemical Physics*, **2000**, 113, 6677-6686	3.9	104
47	Theoretical calculations of excited state absorption. *Physical Chemistry Chemical Physics*, **2000**, 2, 5357-5363	3.6	31
46	Two-photon dissociation and ionization of liquid water studied by femtosecond transient absorption spectroscopy. *Journal of Chemical Physics*, **1999**, 110, 3453-3462	3.9	155
45	Coupled cluster response theory for solvated molecules in equilibrium and nonequilibrium solvation. *Journal of Chemical Physics*, **1999**, 110, 8348-8360	3.9	90
44	A coupled-cluster solvent reaction field method. *Journal of Chemical Physics*, **1999**, 110, 1365-1375	3.9	84

43	The electronic spectrum of pyrrole. *Journal of Chemical Physics*, **1999**, 111, 525-537	3.9	108
42	First-order nonadiabatic coupling matrix elements using coupled cluster methods. I. Theory. *Journal of Chemical Physics*, **1999**, 110, 711-723	3.9	26
41	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	4.4	36
40	Frequency-dependent polarizabilities and first hyperpolarizabilities of CO and H2O from coupled cluster calculations. *Chemical Physics Letters*, **1999**, 305, 147-155	2.5	196
39	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	3.9	80
38	Frequency-dependent second hyperpolarizabilities using coupled cluster cubic response theory. *Chemical Physics Letters*, **1998**, 282, 139-146	2.5	101
37	A second-order doubles correction to excitation energies in the random-phase approximation. *Chemical Physics Letters*, **1998**, 284, 47-55	2.5	36
36	The effect of triple excitations in coupled cluster calculations of frequency-dependent polarizabilities. *Chemical Physics Letters*, **1998**, 292, 437-446	2.5	55
35	Triple excitation effects in coupled-cluster calculations of frequency-dependent hyperpolarizabilities. *Chemical Physics Letters*, **1998**, 296, 117-124	2.5	51
34	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	3.9	120
33	Response functions from Fourier component variational perturbation theory applied to a time-averaged quasienergy. *International Journal of Quantum Chemistry*, **1998**, 68, 1-52	2.1	454
32	The Electronic Spectrum of Furan. *Journal of the American Chemical Society*, **1998**, 120, 3423-3430	16.4	68
31	A coupled cluster study of the 1 1A1g and 1 1B2u states of benzene. *Journal of Chemical Physics*, **1998**, 108, 3987-4001	3.9	64
30	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	3.9	77
29	Integral-direct coupled cluster calculations of frequency-dependent polarizabilities, transition probabilities and excited-state properties. *Journal of Chemical Physics*, **1998**, 108, 2801-2816	3.9	178
28	The benzene–argon complex: A ground and excited state ab initio study. *Journal of Chemical Physics* , **1998**, 108, 2784-2790	3.9	139
27	Coupled cluster response calculations of two-photon transition probability rate constants for helium, neon and argon. *Journal of Chemical Physics*, **1998**, 108, 8355-8359	3.9	38
26	Static and frequency-dependent polarizabilities of excited singlet states using coupled cluster response theory. *Journal of Chemical Physics*, **1998**, 109, 9237-9243	3.9	36

25	Response functions from Fourier component variational perturbation theory applied to a time-averaged quasienergy **1998**, 68, 1		11
24	Response functions from Fourier component variational perturbation theory applied to a time-averaged quasienergy **1998**, 68, 1		21
23	Hyperfine and nuclear quadrupole coupling in chlorine and fluorine dioxides. *Journal of Chemical Physics*, **1997**, 106, 1847-1855	3.9	15
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