Ove Christiansen

List of Publications by Citations

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	The second-order approximate coupled cluster singles and doubles model CC2. *Chemical Physics Letters*, **1995**, 243, 409-418	2.5	1409
203	The Dalton quantum chemistry program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 269-284	7.9	956
202	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
201	Response functions in the CC3 iterative triple excitation model. *Journal of Chemical Physics*, **1995**, 103, 7429-7441	3.9	451
200	The CC3 model: An iterative coupled cluster approach including connected triples. *Journal of Chemical Physics*, **1997**, 106, 1808-1818	3.9	362
199	Vibrational coupled cluster theory. *Journal of Chemical Physics*, **2004**, 120, 2149-59	3.9	248
198	Excitation energies of BH, CH2 and Ne in full configuration interaction and the hierarchy CCS, CC2, CCSD and CC3 of coupled cluster models. *Chemical Physics Letters*, **1995**, 244, 75-82	2.5	217
197	Excitation energies of H2O, N2 and C2 in full configuration interaction and coupled cluster theory. *Chemical Physics Letters*, **1996**, 256, 185-194	2.5	210
196	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
195	Frequency-dependent polarizabilities and first hyperpolarizabilities of CO and H2O from coupled cluster calculations. *Chemical Physics Letters*, **1999**, 305, 147-155	2.5	196
194	Perturbative triple excitation corrections to coupled cluster singles and doubles excitation energies. *Journal of Chemical Physics*, **1996**, 105, 1451-1459	3.9	196
193	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
192	Surprising cases of divergent behavior in Mo/llerPlesset perturbation theory. *Journal of Chemical Physics*, **1996**, 105, 5082-5090	3.9	175
191	A systematic ab initio study of the water dimer in hierarchies of basis sets and correlation models. *Theoretical Chemistry Accounts*, **1997**, 97, 150-157	1.9	173
190	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
189	Large-scale calculations of excitation energies in coupled cluster theory: The singlet excited states of benzene. *Journal of Chemical Physics*, **1996**, 105, 6921-6939	3.9	173
188	MllerPlesset perturbation theory for vibrational wave functions. *Journal of Chemical Physics*, **2003**, 119, 5773-5781	3.9	166

187	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
186	The integral-direct coupled cluster singles and doubles model. *Journal of Chemical Physics*, **1996**, 104, 4157-4165	3.9	146
185	The benzene–argon complex: A ground and excited state ab initio study. *Journal of Chemical Physics* , **1998**, 108, 2784-2790	3.9	139
184	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
183	Excited state coupled cluster methods. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 566-584	7.9	132
182	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
181	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
180	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
179	Frequency-dependent first hyperpolarizabilities using coupled cluster quadratic response theory. *Chemical Physics Letters*, **1997**, 269, 428-434	2.5	119
178	Coupled-cluster response theory for near-edge x-ray-absorption fine structure of atoms and molecules. *Physical Review A*, **2012**, 85,	2.6	117
177	First-order one-electron properties in the integral-direct coupled cluster singles and doubles model. *Journal of Chemical Physics*, **1997**, 107, 849-866	3.9	117
176	A direct atomic orbital driven implementation of the coupled cluster singles and doubles (CCSD) model. *Chemical Physics Letters*, **1994**, 228, 233-238	2.5	115
175	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
174	Linear response functions for coupled cluster/molecular mechanics including polarization interactions. *Journal of Chemical Physics*, **2003**, 118, 1620-1633	3.9	111
173	A second quantization formulation of multimode dynamics. *Journal of Chemical Physics*, **2004**, 120, 2140-8	3.9	108
172	The electronic spectrum of pyrrole. *Journal of Chemical Physics*, **1999**, 111, 525-537	3.9	108
171	The polarizable embedding coupled cluster method. *Journal of Chemical Physics*, **2011**, 134, 104108	3.9	106
170	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

169	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
168	Frequency-dependent second hyperpolarizabilities using coupled cluster cubic response theory. *Chemical Physics Letters*, **1998**, 282, 139-146	2.5	101
167	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
166	Overview of theoretical and computational methods applied to the oxygen-organic molecule photosystem. *Photochemistry and Photobiology*, **2006**, 82, 1136-60	3.6	94
165	Coupled cluster response theory for solvated molecules in equilibrium and nonequilibrium solvation. *Journal of Chemical Physics*, **1999**, 110, 8348-8360	3.9	90
164	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
163	Scrutinizing the effects of polarization in QM/MM excited state calculations. *Physical Chemistry Chemical Physics*, **2011**, 13, 18551-60	3.6	84
162	A coupled-cluster solvent reaction field method. *Journal of Chemical Physics*, **1999**, 110, 1365-1375	3.9	84
161	Spin-orbit coupling constants from coupled-cluster response theory. *Physical Chemistry Chemical Physics*, **2000**, 2, 965-971	3.6	83
160	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
159	Vibrational excitation energies from vibrational coupled cluster response theory. *Journal of Chemical Physics*, **2007**, 126, 204101	3.9	77
158	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
157	On the inherent divergence in the M□ller-Plesset series. The neon atom □a test case. *Chemical Physics Letters*, **1996**, 261, 369-378	2.5	74
156	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
155	Failures of TDDFT in describing the lowest intramolecular charge-transfer excitation in para-nitroaniline. *Molecular Physics*, **2013**, 111, 1235-1248	1.7	71
154	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
153	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
152	Divergence in M□llerPlesset theory: A simple explanation based on a two-state model. *Journal of Chemical Physics*, **2000**, 112, 9736-9748	3.9	71

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150	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
149	Coupled Cluster/Molecular Mechanics Method: Implementation and Application to Liquid Water. *Journal of Physical Chemistry A*, **2003**, 107, 2578-2588	2.8	69
148	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
147	The Electronic Spectrum of Furan. *Journal of the American Chemical Society*, **1998**, 120, 3423-3430	16.4	68
146	PERI-CC2: A Polarizable Embedded RI-CC2 Method. *Journal of Chemical Theory and Computation*, **2012**, 8, 3274-83	6.4	66
145	A theoretical study of the electronic spectrum of water. *Journal of Chemical Physics*, **2000**, 113, 8101-8112	3.9	65
144	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
143	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
142	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
141	Automatic derivation and evaluation of vibrational coupled cluster theory equations. *Journal of Chemical Physics*, **2009**, 131, 234109	3.9	60
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139	Response theory for vibrational wave functions. *Journal of Chemical Physics*, **2005**, 122, 194105	3.9	58
138	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
137	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
136	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
135	The effect of triple excitations in coupled cluster calculations of frequency-dependent polarizabilities. *Chemical Physics Letters*, **1998**, 292, 437-446	2.5	55
134	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

133	Gas phase absorption studies of photoactive yellow protein chromophore derivatives. *Journal of Physical Chemistry A*, **2009**, 113, 9442-9	2.8	52
132	Triple excitation effects in coupled-cluster calculations of frequency-dependent hyperpolarizabilities. *Chemical Physics Letters*, **1998**, 296, 117-124	2.5	51
131	Coupled Cluster Theory with Emphasis on Selected New Developments. *Theoretical Chemistry Accounts*, **2006**, 116, 106-123	1.9	51
130	Automatic generation of potential energy and property surfaces of polyatomic molecules in normal coordinates. *Journal of Chemical Physics*, **2007**, 127, 204106	3.9	51
129	Integral direct calculation of CC2 excitation energies: singlet excited states of benzene. *Chemical Physics Letters*, **1996**, 263, 530-539	2.5	51
128	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
127	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
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125	Linear response functions for a vibrational configuration interaction state. *Journal of Chemical Physics*, **2006**, 125, 214309	3.9	49
124	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
123	Optimized coordinates in vibrational coupled cluster calculations. *Journal of Chemical Physics*, **2014**, 140, 154102	3.9	47
122	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
121	Vibrational coupled cluster response theory: a general implementation. *Journal of Chemical Physics*, **2011**, 134, 054119	3.9	45
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118	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
117	On the coupling strength in potential energy surfaces for vibrational calculations. *Chemical Physics Letters*, **2009**, 483, 138-142	2.5	43
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115	Coupled-cluster theory in a projected atomic orbital basis. *Journal of Chemical Physics*, **2006**, 124, 084103	3.9	42
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113	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
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111	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
110	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
109	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
108	Gaussian process regression to accelerate geometry optimizations relying on numerical differentiation. *Journal of Chemical Physics*, **2018**, 148, 241704	3.9	37
107	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
106	A second-order doubles correction to excitation energies in the random-phase approximation. *Chemical Physics Letters*, **1998**, 284, 47-55	2.5	36
105	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
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100	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
99	Ab initio modeling of excited state absorption of polyenes. *Physical Chemistry Chemical Physics*, **2001**, 3, 2567-2575	3.6	34
98	A variational approach for calculating Franck-Condon factors including mode-mode anharmonic coupling. *Journal of Chemical Physics*, **2006**, 125, 154114	3.9	33

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96	Photoionization cross section by Stieltjes imaging applied to coupled cluster Lanczos pseudo-spectra. *Journal of Chemical Physics*, **2013**, 139, 094103	3.9	31
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93	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
92	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
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90	Machine learning for potential energy surfaces: An extensive database and assessment of methods. *Journal of Chemical Physics*, **2019**, 150, 244113	3.9	29
89	Approximate high mode coupling potentials using Gaussian process regression and adaptive density guided sampling. *Journal of Chemical Physics*, **2019**, 150, 131102	3.9	28
88	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
87	Variational calculation of static and dynamic vibrational nonlinear optical properties. *Journal of Chemical Physics*, **2007**, 127, 084118	3.9	28
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76	Linear response coupled cluster study of the benzene excimer. *Chemical Physics Letters*, **2009**, 482, 44-49	2.5	23
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74	Automatic determination of important mode-mode correlations in many-mode vibrational wave functions. *Journal of Chemical Physics*, **2015**, 142, 144115	3.9	22
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72	Response functions from Fourier component variational perturbation theory applied to a time-averaged quasienergy **1998**, 68, 1		21
71	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
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68	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
67	Lanczos-driven coupled-cluster damped linear response theory for molecules in polarizable environments. *Journal of Chemical Physics*, **2014**, 141, 244107	3.9	19
66	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
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64	Tensor decomposition and vibrational coupled cluster theory. *Journal of Physical Chemistry A*, **2013**, 117, 7267-79	2.8	18
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56	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
55	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
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45	A Lanczos-chain driven approach for calculating damped vibrational configuration interaction response functions. *Journal of Chemical Physics*, **2010**, 133, 114102	3.9	13
44	Polarizable Embedded RI-CC2 Method for Two-Photon Absorption Calculations. *Journal of Chemical Theory and Computation*, **2015**, 11, 3669-78	6.4	11

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