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	The second-order approximate coupled cluster singles and doubles model CC2. Chemical Physics Letters, 1995, 243, 409-418.	1.2	1,564
2	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	6.2	1,166
3	Response functions in the CC3 iterative triple excitation model. Journal of Chemical Physics, 1995, 103, 7429-7441.	1.2	498
4	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
5	The CC3 model: An iterative coupled cluster approach including connected triples. Journal of Chemical Physics, 1997, 106, 1808-1818.	1.2	412
6	Vibrational coupled cluster theory. Journal of Chemical Physics, 2004, 120, 2149-2159.	1.2	289
7	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.	1.2	232
8	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
9	Frequency-dependent polarizabilities and first hyperpolarizabilities of CO and H2O from coupled cluster calculations. Chemical Physics Letters, 1999, 305, 147-155.	1.2	219
10	Excitation energies of H2O, N2 and C2 in full configuration interaction and coupled cluster theory. Chemical Physics Letters, 1996, 256, 185-194.	1.2	218
11	Perturbative triple excitation corrections to coupled cluster singles and doubles excitation energies. Journal of Chemical Physics, 1996, 105, 1451-1459.	1.2	211
12	Surprising cases of divergent behavior in Mo/llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 1996, 105, 5082-5090.	1.2	192
13	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
14	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
15	MÃllerâ€“Plesset perturbation theory for vibrational wave functions. Journal of Chemical Physics, 2003, 119, 5773-5781.	1.2	186
16	A systematic ab initio study of the water dimer in hierarchies of basis sets and correlation models. Theoretical Chemistry Accounts, 1997, 97, 150-157.	0.5	184
17	Largeâ€scale calculations of excitation energies in coupled cluster theory: The singlet excited states of benzene. Journal of Chemical Physics, 1996, 105, 6921-6939.	1.2	182
18	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

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19	Excited state coupled cluster methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 566-584.	6.2	165
20	The integralâ€direct coupled cluster singles and doubles model. Journal of Chemical Physics, 1996, 104, 4157-4165.	1.2	154
21	The benzeneâ€“argon complex: A ground and excited state ab initio study. Journal of Chemical Physics, 1998, 108, 2784-2790.	1.2	144
22	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
23	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
24	Coupled-cluster response theory for near-edge x-ray-absorption fine structure of atoms and molecules. Physical Review A, 2012, 85, .	1.0	137
25	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
26	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
27	A second quantization formulation of multimode dynamics. Journal of Chemical Physics, 2004, 120, 2140-2148.	1.2	127
28	A direct atomic orbital driven implementation of the coupled cluster singles and doubles (CCSD) model. Chemical Physics Letters, 1994, 228, 233-238.	1.2	126
29	Frequency-dependent first hyperpolarizabilities using coupled cluster quadratic response theory. Chemical Physics Letters, 1997, 269, 428-434.	1.2	125
30	First-order one-electron properties in the integral-direct coupled cluster singles and doubles model. Journal of Chemical Physics, 1997, 107, 849-866.	1.2	122
31	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
32	Selected new developments in vibrational structure theory: potential construction and vibrational wave function calculations. Physical Chemistry Chemical Physics, 2012, 14, 6672.	1.3	121
33	The electronic spectrum of pyrrole. Journal of Chemical Physics, 1999, 111, 525-537.	1.2	117
34	Linear response functions for coupled cluster/molecular mechanics including polarization interactions. Journal of Chemical Physics, 2003, 118, 1620-1633.	1.2	117
35	The polarizable embedding coupled cluster method. Journal of Chemical Physics, 2011, 134, 104108.	1.2	117
36	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

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37	Frequency-dependent second hyperpolarizabilities using coupled cluster cubic response theory. Chemical Physics Letters, 1998, 282, 139-146.	1.2	108
38	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
39	Overview of Theoretical and Computational Methods Applied to the Oxygenâ€“Organic Molecule Photosystem. Photochemistry and Photobiology, 2006, 82, 1136.	1.3	104
40	Coupled cluster response theory for solvated molecules in equilibrium and nonequilibrium solvation. Journal of Chemical Physics, 1999, 110, 8348-8360.	1.2	99
41	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
42	Spin-orbit coupling constants from coupled-cluster response theory. Physical Chemistry Chemical Physics, 2000, 2, 965-971.	1.3	97
43	Scrutinizing the effects of polarization in QM/MM excited state calculations. Physical Chemistry Chemical Physics, 2011, 13, 18551.	1.3	94
44	A coupled-cluster solvent reaction field method. Journal of Chemical Physics, 1999, 110, 1365-1375.	1.2	93
45	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
46	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
47	Vibrational excitation energies from vibrational coupled cluster response theory. Journal of Chemical Physics, 2007, 126, 204101.	1.2	84
48	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
49	On the inherent divergence in the MÃ¸ller-Plesset series. The neon atom â€" a test case. Chemical Physics Letters, 1996, 261, 369-378.	1.2	79
50	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
51	Failures of TDDFT in describing the lowest intramolecular charge-transfer excitation in para-nitroaniline. Molecular Physics, 2013, 111, 1235-1248.	0.8	79
52	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
53	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
54	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

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55	PERIâ€“CC2: A Polarizable Embedded RI-CC2 Method. Journal of Chemical Theory and Computation, 2012, 8, 3274-3283.	2.3	75
56	The Electronic Spectrum of Furan. Journal of the American Chemical Society, 1998, 120, 3423-3430.	6.6	74
57	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
58	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
59	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
60	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
61	Coupled Cluster/Molecular Mechanics Method:â€‰ Implementation and Application to Liquid Water. Journal of Physical Chemistry A, 2003, 107, 2578-2588.	1.1	70
62	New Formulation and Implementation of Vibrational Self-Consistent Field Theory. Journal of Chemical Theory and Computation, 2010, 6, 235-248.	2.3	69
63	A theoretical study of the electronic spectrum of water. Journal of Chemical Physics, 2000, 113, 8101-8112.	1.2	68
64	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
65	Automatic derivation and evaluation of vibrational coupled cluster theory equations. Journal of Chemical Physics, 2009, 131, 234109.	1.2	66
66	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
67	The effect of triple excitations in coupled cluster calculations of frequency-dependent polarizabilities. Chemical Physics Letters, 1998, 292, 437-446.	1.2	61
68	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
69	â€‡Response theory for vibrational wave functions. Journal of Chemical Physics, 2005, 122, 194105.	1.2	60
70	Coupled Cluster Theory with Emphasis on Selected New Developments. Theoretical Chemistry Accounts, 2006, 116, 106-123.	0.5	59
71	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
72	Triple excitation effects in coupled-cluster calculations of frequency-dependent hyperpolarizabilities. Chemical Physics Letters, 1998, 296, 117-124.	1.2	56

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73	Gas Phase Absorption Studies of Photoactive Yellow Protein Chromophore Derivatives. Journal of Physical Chemistry A, 2009, 113, 9442-9449.	1.1	56
74	Optimized coordinates in vibrational coupled cluster calculations. Journal of Chemical Physics, 2014, 140, .	1.2	56
75	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
76	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
77	Automatic generation of potential energy and property surfaces of polyatomic molecules in normal coordinates. Journal of Chemical Physics, 2007, 127, 204106.	1.2	54
78	Gaussian process regression to accelerate geometry optimizations relying on numerical differentiation. Journal of Chemical Physics, 2018, 148, 241704.	1.2	54
79	Integral direct calculation of CC2 excitation energies: singlet excited states of benzene. Chemical Physics Letters, 1996, 263, 530-539.	1.2	53
80	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
81	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
82	Vibrational coupled cluster response theory: A general implementation. Journal of Chemical Physics, 2011, 134, 054119.	1.2	52
83	Cauchy moments and dispersion coefficients using coupled cluster linear response theory. Journal of Chemical Physics, 1997, 107, 10592-10598.	1.2	51
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, 1430-1440.	1.1	51
85	Linear response functions for a vibrational configuration interaction state. Journal of Chemical Physics, 2006, 125, 214309.	1.2	51
86	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
87	Equilibrium geometries of cyclic SiC3 isomers. Journal of Chemical Physics, 2001, 114, 2993-2995.	1.2	50
88	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
89	On the coupling strength in potential energy surfaces for vibrational calculations. Chemical Physics Letters, 2009, 483, 138-142.	1.2	45
90	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

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91	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
92	Coupled-cluster theory in a projected atomic orbital basis. Journal of Chemical Physics, 2006, 124, 084103.	1.2	44
93	Coupled cluster response calculations of two-photon transition probability rate constants for helium, neon and argon. Journal of Chemical Physics, 1998, 108, 8355-8359.	1.2	43
94	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
95	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
96	Linear-scaling generation of potential energy surfaces using a double incremental expansion. Journal of Chemical Physics, 2016, 145, .	1.2	43
97	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
98	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
99	Machine learning for potential energy surfaces: An extensive database and assessment of methods. Journal of Chemical Physics, 2019, 150, 244113.	1.2	42
100	Photoabsorption studies of neutral green fluorescent protein model chromophores in vacuo. Physical Chemistry Chemical Physics, 2009, 11, 9996.	1.3	41
101	A second-order doubles correction to excitation energies in the random-phase approximation. Chemical Physics Letters, 1998, 284, 47-55.	1.2	39
102	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
103	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
104	Static and frequency-dependent polarizabilities of excited singlet states using coupled cluster response theory. Journal of Chemical Physics, 1998, 109, 9237-9243.	1.2	38
105	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
106	Theoretical calculations of excited state absorption. Physical Chemistry Chemical Physics, 2000, 2, 5357-5363.	1.3	37
107	A CC2 dielectric continuum model and a CC2 molecular mechanics model. Molecular Physics, 2003, 101, 2055-2071.	0.8	37
108	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

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109	Hybrid Optimized and Localized Vibrational Coordinates. Journal of Physical Chemistry A, 2015, 119, 11007-11021.	1.1	37
110	A variational approach for calculating Franck-Condon factors including mode-mode anharmonic coupling. Journal of Chemical Physics, 2006, 125, 154114.	1.2	36
111	Approximate high mode coupling potentials using Gaussian process regression and adaptive density guided sampling. Journal of Chemical Physics, 2019, 150, 131102.	1.2	36
112	Ab initio modeling of excited state absorption of polyenes. Physical Chemistry Chemical Physics, 2001, 3, 2567-2575.	1.3	35
113	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
114	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
115	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
116	Photoionization cross section by Stieltjes imaging applied to coupled cluster Lanczos pseudo-spectra. Journal of Chemical Physics, 2013, 139, 094103.	1.2	33
117	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
118	FALCON: A method for flexible adaptation of local coordinates of nuclei. Journal of Chemical Physics, 2016, 144, 074108.	1.2	32
119	Computational screening of one- and two-photon spectrally tuned channelrhodopsin mutants. Physical Chemistry Chemical Physics, 2013, 15, 7567.	1.3	31
120	First-order nonadiabatic coupling matrix elements using coupled cluster methods. I. Theory. Journal of Chemical Physics, 1999, 110, 711-723.	1.2	30
121	General biorthogonal projected bases as applied to second-order MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2007, 127, 074106.	1.2	30
122	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
123	Variational calculation of static and dynamic vibrational nonlinear optical properties. Journal of Chemical Physics, 2007, 127, 084118.	1.2	29
124	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
125	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
126	A simple state-average procedure determining optimal coordinates for anharmonic vibrational calculations. Chemical Physics Letters, 2014, 610-611, 288-297.	1.2	29

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127	Automatic determination of important modeâ€“mode correlations in many-mode vibrational wave functions. Journal of Chemical Physics, 2015, 142, 144115.	1.2	29
128	Linear response coupled cluster study of the benzene excimer. Chemical Physics Letters, 2009, 482, 44-49.	1.2	28
129	Vibrational absorption spectra calculated from vibrational configuration interaction response theory using the Lanczos method. Journal of Chemical Physics, 2010, 132, 164105.	1.2	26
130	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
131	Nuclear magnetic shielding constants in the CC2 model. Chemical Physics Letters, 1997, 266, 53-60.	1.2	25
132	Electronic excitation energies of pyrimidine studied using coupled cluster response theory. Physical Chemistry Chemical Physics, 2001, 3, 730-740.	1.3	25
133	Tensor Decomposition and Vibrational Coupled Cluster Theory. Journal of Physical Chemistry A, 2013, 117, 7267-7279.	1.1	24
134	Accurate Nonlinear Optical Properties for Small Molecules. Challenges and Advances in Computational Chemistry and Physics, 2006, , 51-99.	0.6	23
135	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
136	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
137	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
138	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
139	Response functions from Fourier component variational perturbation theory applied to a timeâ€averaged quasienergy. International Journal of Quantum Chemistry, 1998, 68, 1-52.	1.0	21
140	Triple excitation effects in coupled cluster calculations of Verdet constants. Chemical Physics Letters, 2000, 330, 463-470.	1.2	20
141	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
142	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
143	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
144	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

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145	Anharmonic vibrational spectra from double incremental potential energy and dipole surfaces. Physical Chemistry Chemical Physics, 2018, 20, 3445-3456.	1.3	20
146	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
147	Lanczos-driven coupledâ€“cluster damped linear response theory for molecules in polarizable environments. Journal of Chemical Physics, 2014, 141, 244107.	1.2	19
148	The hyperpolarizability of neon revisited. Chemical Physics Letters, 1993, 207, 367-371.	1.2	18
149	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
150	Uptake of Phenol on Aerosol Particlesâ€. Journal of Physical Chemistry A, 2006, 110, 660-670.	1.1	18
151	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
152	An improved value of the nuclear quadrupole moment of the 197 keV I = 52 excited state of 19F. Chemical Physics Letters, 1997, 271, 273-279.	1.2	17
153	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
154	Tensor decomposition techniques in the solution of vibrational coupled cluster response theory eigenvalue equations. Journal of Chemical Physics, 2015, 142, 024105.	1.2	17
155	Tensor-decomposed vibrational coupled-cluster theory: Enabling large-scale, highly accurate vibrational-structure calculations. Journal of Chemical Physics, 2018, 148, 024103.	1.2	17
156	A Gaussian process regression adaptive density guided approach for potential energy surface construction. Journal of Chemical Physics, 2020, 153, 064105.	1.2	17
157	Hyperfine and nuclear quadrupole coupling in chlorine and fluorine dioxides. Journal of Chemical Physics, 1997, 106, 1847-1855.	1.2	16
158	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
159	Theory of hyperfine coupling constants of solvated molecules: Applications involving methyl and ClO2 radicals in different solvents. Journal of Chemical Physics, 1996, 104, 629-635.	1.2	15
160	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
161	A Lanczos-chain driven approach for calculating damped vibrational configuration interaction response functions. Journal of Chemical Physics, 2010, 133, 114102.	1.2	15
162	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

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163	Vibrationally resolved emission spectra of luminescent conjugated oligothiophenes from anharmonic calculations. Physical Chemistry Chemical Physics, 2019, 21, 17410-17422.	1.3	15
164	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
165	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
166	Fast Photodynamics of Aqueous Formic Acid. Journal of Physical Chemistry A, 2004, 108, 7483-7489.	1.1	12
167	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
168	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
169	Polarizable Embedded RI-CC2 Method for Two-Photon Absorption Calculations. Journal of Chemical Theory and Computation, 2015, 11, 3669-3678.	2.3	12
170	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
171	Exponential parameterization of wave functions for quantum dynamics: Time-dependent Hartree in second quantization. Journal of Chemical Physics, 2018, 149, 134110.	1.2	12
172	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
173	Quantum embedding description of the Anderson lattice model with the ghost Gutzwiller approximation. Physical Review B, 2021, 104, .	1.1	11
174	Response functions from Fourier component variational perturbation theory applied to a time-averaged quasienergy. , 1998, 68, 1.		11
175	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
176	Vibrational contributions to cubic response functions from vibrational configuration interaction response theory. Journal of Chemical Physics, 2011, 135, 154107.	1.2	10
177	Identifying the Hamiltonian structure in linear response theory. Journal of Chemical Physics, 2014, 140, 224103.	1.2	10
178	Time-dependent vibrational coupled cluster with variationally optimized time-dependent basis sets. Journal of Chemical Physics, 2020, 153, 174108.	1.2	10
179	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
180	NMR properties of N3â¯. A comparison of theory and experiment. Chemical Physics Letters, 1995, 243, 144-150.	1.2	9

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181	Computation of expectation values from vibrational coupled-cluster at the two-mode coupling level. Journal of Chemical Physics, 2011, 134, 154101.	1.2	9
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