Sonia Coriani

List of Publications by Year
in descending order

179 papers	8,197 citations	76326 40 h-index	56724 83 g-index
229 all docs	229 docs citations	229 times ranked	5137 citing authors

#	Article	IF	Citations
1	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	14.6	1,166
2	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. Journal of Chemical Physics, 2020, 152, 184107.	3.0	616
3	Recent Advances in Wave Function-Based Methods of Molecular-Property Calculations. Chemical Reviews, 2012, 112, 543-631.	47.7	549
4	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
5	On CHF calculations of second-order magnetic properties using the method of continuous transformation of origin of the current density. Theoretica Chimica Acta, 1994, 89, 181-192.	0.8	206
6	Communication: X-ray absorption spectra and core-ionization potentials within a core-valence separated coupled cluster framework. Journal of Chemical Physics, 2015, 143, 181103.	3.0	162
7	The Equilibrium Structure of Ferrocene. ChemPhysChem, 2006, 7, 245-249.	2.1	149
8	Probing ultrafast Ï€Ï€*/nÏ€* internal conversion in organic chromophores via K-edge resonant absorption. Nature Communications, 2017, 8, 29.	12.8	144
9	New and Efficient Equation-of-Motion Coupled-Cluster Framework for Core-Excited and Core-Ionized States. Journal of Chemical Theory and Computation, 2019, 15, 3117-3133.	5.3	139
10	Coupled-cluster response theory for near-edge x-ray-absorption fine structure of atoms and molecules. Physical Review A, 2012, 85, .	2.5	137
11	The accuracy ofab initiomolecular geometries for systems containing second-row atoms. Journal of Chemical Physics, 2005, 123, 184107.	3.0	125
12	A density matrix-based quasienergy formulation of the Kohnâ€“Sham density functional response theory using perturbation- and time-dependent basis sets. Journal of Chemical Physics, 2008, 129, 214108.	3.0	99
13	Asymmetric-Lanczos-Chain-Driven Implementation of Electronic Resonance Convergent Coupled-Cluster Linear Response Theory. Journal of Chemical Theory and Computation, 2012, 8, 1616-1628.	5.3	98
14	Optical Rotation Calculation of a Highly Flexible Molecule:Â The Case of Paraconic Acid. Journal of Physical Chemistry A, 2005, 109, 1449-1453.	2.5	91
15	Linear-scaling implementation of molecular response theory in self-consistent field electronic-structure theory. Journal of Chemical Physics, 2007, 126, 154108.	3.0	87
16	Accurate calculation and modeling of the adiabatic connection in density functional theory. Journal of Chemical Physics, 2010, 132, 164115.	3.0	86
17	On the molecular electric quadrupole moment and the electric-field-gradient-induced birefringence of CO2 and CS2. Chemical Physics Letters, 2000, 326, 269-276.	2.6	83
18	Linear-scaling implementation of molecular electronic self-consistent field theory. Journal of Chemical Physics, 2007, 126, 114110.	3.0	78

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19	e T 1.0: An open source electronic structure program with emphasis on coupled cluster and multilevel methods. Journal of Chemical Physics, 2020, 152, 184103.	3.0	68
20	Ab initio determinations of magnetic circular dichroism. Chemical Physics Letters, 1999, 300, 61-68.	2.6	66
21	Coupled cluster calculations of the ground state potential and interaction induced electric properties of the mixed dimers of helium, neon and argon. Molecular Physics, 2004, 102, 101-110.	1.7	65
22	Gauge-origin independent magneto-optical activity within coupled cluster response theory. Journal of Chemical Physics, 2000, 113, 3561-3572.	3.0	64
23	The calculation of adiabatic-connection curves from full configuration-interaction densities: Two-electron systems. Journal of Chemical Physics, 2009, 130, 104111.	3.0	64
24	Complex polarization propagator calculations of magnetic circular dichroism spectra. Journal of Chemical Physics, 2008, 128, 094103.	3.0	63
25	Polarizable continuum model study of solvent effects on electronic circular dichroism parameters. Journal of Chemical Physics, 2005, 122, 024106.	3.0	58
26	A Lagrangian, integral-density direct formulation and implementation of the analytic CCSD and CCSD(T) gradients. Journal of Chemical Physics, 2003, 118, 2985-2998.	3.0	57
27	The molecular electric quadrupole moment of N2. Chemical Physics Letters, 1998, 294, 292-296.	2.6	56
28	The A and B Terms of Magnetic Circular Dichroism Revisited. Journal of Physical Chemistry A, 2008, 112, 9615-9618.	2.5	55
29	Benchmark Calculations of K-Edge Ionization Energies for First-Row Elements Using Scalar-Relativistic Coreâ€“Valence-Separated Equation-of-Motion Coupled-Cluster Methods. Journal of Chemical Theory and Computation, 2019, 15, 1642-1651.	5.3	54
30	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.	3.0	53
31	Ab initiostudy of magnetochiral birefringence. Journal of Chemical Physics, 2002, 117, 6417-6428.	3.0	51
32	Dyson orbitals within the fc-CVS-EOM-CCSD framework: theory and application to X-ray photoelectron spectroscopy of ground and excited states. Physical Chemistry Chemical Physics, 2020, 22, 2693-2703.	2.8	48
33	Equation-of-Motion Coupled-Cluster Theory to Model L-Edge X-ray Absorption and Photoelectron Spectra. Journal of Physical Chemistry Letters, 2020, 11, 8314-8321.	4.6	46
34	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.	3.0	45
35	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. Journal of Chemical Physics, 2020, 152, 214115.	3.0	45
36	Jones birefringence in gases:Ab initioelectron correlated results for atoms and linear molecules. Journal of Chemical Physics, 2003, 119, 11064-11079.	3.0	42

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37	Hartree-Fock and Kohn-Sham time-dependent response theory in a second-quantization atomic-orbital formalism suitable for linear scaling. Journal of Chemical Physics, 2008, 129, 054106.	3.0	42
38	Spin flipping in ring-coupled-cluster-doubles theory. Chemical Physics Letters, 2011, 510, 147-153.	2.6	42
39	How to stay out of trouble in RIXS calculations within equation-of-motion coupled-cluster damped response theory? Safe hitchhiking in the excitation manifold by means of coreâ€“valence separation. Physical Chemistry Chemical Physics, 2020, 22, 2629-2641.	2.8	42
40	Coupled cluster investigation of the electric-field-gradient-induced birefringence of H2, N2, C2H2, and CH4. Journal of Chemical Physics, 1998, 109, 7176-7184.	3.0	40
41	Resonant Inelastic X-ray Scattering and Nonesonant X-ray Emission Spectra from Coupled-Cluster (Damped) Response Theory. Journal of Chemical Theory and Computation, 2019, 15, 520-528.	5.3	40
42	MCSCF calculations of hypermagnetizabilities and nuclear shielding polarizabilities of CO and CH₄. Molecular Physics, 1996, 88, 931-947.	1.7	39
43	On the basis set selection for calculations of core-level states: different strategies to balance cost and accuracy. Molecular Physics, 2020, 118, e1769872.	1.7	39
44	Static and frequency-dependent polarizabilities of excited singlet states using coupled cluster response theory. Journal of Chemical Physics, 1998, 109, 9237-9243.	3.0	38
45	Communication: Analytic gradients in the random-phase approximation. Journal of Chemical Physics, 2013, 139, 081101.	3.0	38
46	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.	3.0	37
47	Implementation of the incremental scheme for one-electron first-order properties in coupled-cluster theory. Journal of Chemical Physics, 2009, 131, 154102.	3.0	37
48	Gauge-Origin Independent Formulation and Implementation of Magneto-Optical Activity within Atomic-Orbital-Density Based Hartreeâ^'Fock and Kohnâ^'Sham Response Theories. Journal of Chemical Theory and Computation, 2009, 5, 1997-2020.	5.3	37
49	XABOOM: An X-ray Absorption Benchmark of Organic Molecules Based on Carbon, Nitrogen, and Oxygen 1s â†' Ï€* Transitions. Journal of Chemical Theory and Computation, 2021, 17, 1618-1637.	5.3	37
50	Ab initio study of the electric-field-gradient-induced birefringence of a polar molecule: CO. Journal of Chemical Physics, 2000, 113, 3077-3087.	3.0	36
51	Relative Stability of the L_a and L_b Excited States in Adenine and Guanine: Direct Evidence from TD-DFT Calculations of MCD Spectra. Journal of Physical Chemistry Letters, 2014, 5, 1806-1811.	4.6	36
52	Near-Edge X-ray Absorption Fine Structure within Multilevel Coupled Cluster Theory. Journal of Chemical Theory and Computation, 2016, 12, 2633-2643.	5.3	35
53	Photoionization cross section by Stieltjes imaging applied to coupled cluster Lanczos pseudo-spectra. Journal of Chemical Physics, 2013, 139, 094103.	3.0	33
54	Molecular inner-shell photoabsorption/photoionization cross sections at core-valence-separated coupled cluster level: Theory and examples. Journal of Chemical Physics, 2019, 150, 224104.	3.0	33

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55	On the molecular electric quadrupole moment of C2H2. Chemical Physics Letters, 1999, 303, 408-412.	2.6	32
56	Solvent effects on the conformational distribution and optical rotation of Î³-methyl paraconic acids and esters. Chirality, 2006, 18, 357-369.	2.6	32
57	Dynamical photoionization observables of the CS molecule: The role of electron correlation. Journal of Chemical Physics, 2014, 140, 204304.	3.0	32
58	Time-resolved near-edge X-ray absorption fine structure of pyrazine from electronic structure and nuclear wave packet dynamics simulations. Journal of Chemical Physics, 2019, 151, 124114.	3.0	32
59	An IEF-PCM study of solvent effects on the Faraday $${mathcal{B}}$$ term of MCD. Theoretical Chemistry Accounts, 2008, 119, 231-244.	1.4	31
60	Coreâ€“valence-separated coupled-cluster-singles-and-doubles complex-polarization-propagator approach to X-ray spectroscopies. Physical Chemistry Chemical Physics, 2020, 22, 2642-2647.	2.8	31
61	Interplay of Open-Shell Spin-Coupling and Jahnâ€“Teller Distortion in Benzene Radical Cation Probed by X-ray Spectroscopy. Journal of Physical Chemistry A, 2020, 124, 9532-9541.	2.5	31
62	Density-functional and electron correlated study of five linear birefringencesâ€”Kerr, Cottonâ€“Mouton, Buckingham, Jones, and magnetoelectricâ€”in gaseous benzene. Journal of Chemical Physics, 2004, 121, 8814-8830.	3.0	30
63	Range-dependent adiabatic connections. Journal of Chemical Physics, 2010, 133, 164112.	3.0	30
64	Requirements of first-principles calculations of X-ray absorption spectra of liquid water. Physical Chemistry Chemical Physics, 2016, 18, 566-583.	2.8	30
65	An analysis of the performance of coupled cluster methods for K-edge core excitations and ionizations using standard basis sets. Advances in Quantum Chemistry, 2019, 79, 241-261.	0.8	30
66	Cotton-Mouton effect and shielding polarizabilities of ethylene: An MCSCF study. Chemical Physics, 1997, 216, 53-66.	1.9	29
67	A closed-shell coupled-cluster treatment of the Breitâ€“Pauli first-order relativistic energy correction. Journal of Chemical Physics, 2004, 121, 6591-6598.	3.0	29
68	Molecular response properties in equation of motion coupled cluster theory: A time-dependent perspective. Journal of Chemical Physics, 2016, 144, 024102.	3.0	29
69	X-ray transient absorption reveals the 1Au (nÏ€*) state of pyrazine in electronic relaxation. Nature Communications, 2021, 12, 5003.	12.8	29
70	Gauge-Origin-Independent Coupled Cluster Singles and Doubles Calculation of Magnetic Circular Dichroism of Azabenzenes and Phosphabenzene Using London Orbitals. Journal of Physical Chemistry A, 2007, 111, 11278-11286.	2.5	28
71	An Atomic-Orbital-Based Lagrangian Approach for Calculating Geometric Gradients of Linear Response Properties. Journal of Chemical Theory and Computation, 2010, 6, 1028-1047.	5.3	28
72	Resonant Inelastic X-Ray Scattering Reveals Hidden Local Transitions of the Aqueous OH Radical. Physical Review Letters, 2020, 124, 236001.	7.8	28

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73	Density-functional theory study of electric and magnetic properties of hexafluorobenzene in the vapor phase. Journal of Chemical Physics, 2005, 122, 234314.	3.0	27
74	Ab initio calculation of magnetic circular dichroism. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 443-455.	14.6	27
75	A theoretical and experimental benchmark study of core-excited states in nitrogen. Journal of Chemical Physics, 2018, 148, 064106.	3.0	27
76	The electric-field-gradient-induced birefringence of Helium, Neon, Argon, and SF6. Journal of Chemical Physics, 1999, 111, 7828-7836.	3.0	26
77	Birefringences: A Challenge for Both Theory and Experiment. Advances in Quantum Chemistry, 2005, , 143-184.	0.8	26
78	Accurate Description of Photoionization Dynamical Parameters. Journal of Physical Chemistry Letters, 2020, 11, 5330-5337.	4.6	26
79	Relativistic EOM-CCSD for Core-Excited and Core-Ionized State Energies Based on the Four-Component Diracâ€“Coulomb(â^’Gaunt) Hamiltonian. Journal of Chemical Theory and Computation, 2021, 17, 3583-3598.	5.3	26
80	Critical analysis of the spin-rotation constants of CF2 and CCl2: A theoretical investigation. Chemical Physics Letters, 2005, 409, 118-123.	2.6	24
81	Coupled cluster study of the x-ray absorption spectra of formaldehyde derivatives at the oxygen, carbon, and fluorine K-edges. Journal of Chemical Physics, 2019, 151, 064107.	3.0	24
82	UV Absorption and Magnetic Circular Dichroism Spectra of Purine, Adenine, and Guanine: A Coupled Cluster Study in Vacuo and in Aqueous Solution. Journal of Chemical Theory and Computation, 2019, 15, 1242-1254.	5.3	24
83	Table-Top X-ray Spectroscopy of Benzene Radical Cation. Journal of Physical Chemistry A, 2020, 124, 9524-9531.	2.5	24
84	A combined experimental and computational strategy in the assignment of absolute configurations of 4-methyl-5-oxo-tetrahydrofuran-3-carboxylic acids and their esters. Tetrahedron: Asymmetry, 2005, 16, 3011-3023.	1.8	23
85	Combined density functional/polarizable continuum model study of magnetochiral birefringence: Can theory and experiment be brought to agreement?. Journal of Chemical Physics, 2006, 125, 234105.	3.0	23
86	Accurate Nonlinear Optical Properties for Small Molecules. Challenges and Advances in Computational Chemistry and Physics, 2006, , 51-99.	0.6	23
87	Analytical calculations of frequency-dependent hypermagnetizabilities and Cottonâ€“Mouton constants using London atomic orbitals. Journal of Chemical Physics, 2008, 129, 164110.	3.0	23
88	Coupled cluster calculations of Verdet constants. Chemical Physics Letters, 1997, 281, 445-451.	2.6	22
89	MCSCF polarizability and hyperpolarizabilities of HCl and HBr. Chemical Physics Letters, 1998, 288, 677-688.	2.6	21
90	The effect of triple excitations in coupled cluster calculations of Raman scattering cross-sections. Chemical Physics Letters, 2002, 355, 327-338.	2.6	21

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91	First-order relativistic corrections to response properties: the hyperpolarizability of the Ne atom. Journal of Physics B: Atomic, Molecular and Optical Physics, 2004, 37, 3753-3763.	1.5	21
92	Dispersion interactions in density-functional theory: An adiabatic-connection analysis. Journal of Chemical Physics, 2011, 135, 194109.	3.0	21
93	TD-DFT Investigation of the Magnetic Circular Dichroism Spectra of Some Purine and Pyrimidine Bases of Nucleic Acids. Journal of Physical Chemistry A, 2015, 119, 5476-5489.	2.5	21
94	Coupled Cluster Study of Photoionization and Photodetachment Cross Sections. Journal of Chemical Theory and Computation, 2016, 12, 4440-4459.	5.3	21
95	The Cotton-Mouton effect of liquid water. Part I: The dielectric continuum model. Journal of Chemical Physics, 1997, 107, 894-901.	3.0	20
96	The Cottonâ€“Mouton effect of liquid water. Part II: The semi-continuum model. Journal of Chemical Physics, 1998, 108, 599-603.	3.0	20
97	Triple excitation effects in coupled cluster calculations of Verdet constants. Chemical Physics Letters, 2000, 330, 463-470.	2.6	20
98	Nuclear spin circular dichroism. Journal of Chemical Physics, 2014, 140, 134103.	3.0	20
99	From Pentalene to Dicyclopenta[b,g]naphthalene, or the Change towards Delocalized Structures. ChemPhysChem, 2006, 7, 240-244.	2.1	19
100	Analytic ab initio calculations of coherent anti-Stokes Raman scattering (CARS). Physical Chemistry Chemical Physics, 2009, 11, 2293.	2.8	19
101	Lanczos-driven coupledâ€“cluster damped linear response theory for molecules in polarizable environments. Journal of Chemical Physics, 2014, 141, 244107.	3.0	19
102	The nuclear-spin-rotation constants of HCY, HSiY, and SiY2 (Y=F, Cl): An ab initio study. Journal of Chemical Physics, 2006, 124, 064302.	3.0	18
103	Picosecond timescale tracking of pentacene triplet excitons with chemical sensitivity. Communications Physics, 2019, 2, .	5.3	18
104	An assessment of different electronic structure approaches for modeling time-resolved x-ray absorption spectroscopy. Structural Dynamics, 2021, 8, 024101.	2.3	18
105	Comparison of standard and damped response formulations of magnetic circular dichroism. Journal of Chemical Physics, 2011, 135, 024112.	3.0	17
106	The magnetic circular dichroism spectrum of the C₆₀ fullerene. Molecular Physics, 2013, 111, 1401-1404.	1.7	17
107	Variational response-function formulation of vibrational circular dichroism. Physical Chemistry Chemical Physics, 2011, 13, 4224.	2.8	16
108	The Cottonâ€“Mouton effect of gaseous CO2, N2O, OCS, and CS2. A cubic response multiconfigurational self-consistent field study. Journal of Chemical Physics, 2001, 114, 8372-8381.	3.0	15

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109	A coupled cluster response study of the electric dipole polarizability, first and second hyperpolarizabilities of HCl. Physical Chemistry Chemical Physics, 2002, 4, 2884-2890.	2.8	15
110	A computational protocol for the study of circularly polarized phosphorescence and circular dichroism in spin-forbidden absorption. Physical Chemistry Chemical Physics, 2015, 17, 19079-19086.	2.8	15
111	Optical absorption and magnetic circular dichroism spectra of thiouracils: a quantum mechanical study in solution. Photochemical and Photobiological Sciences, 2017, 16, 1415-1423.	2.9	15
112	Excited-State Absorption of Uracil in the Gas Phase: Mapping the Main Decay Paths by Different Electronic Structure Methods. Journal of Chemical Theory and Computation, 2021, 17, 1638-1652.	5.3	15
113	Analytic calculations of nonlinear mixed electric and magnetic frequency-dependent molecular properties using London atomic orbitals: Buckingham birefringence. Physical Chemistry Chemical Physics, 2009, 11, 816-825.	2.8	14
114	X-ray and UV Spectra of Glycine within Coupled Cluster Linear Response Theory. Journal of Physical Chemistry A, 2019, 123, 9701-9711.	2.5	14
115	Capturing Correlation Effects on Photoionization Dynamics. Journal of Chemical Theory and Computation, 2021, 17, 5064-5079.	5.3	14
116	Simulating weak-field attosecond processes with a Lanczos reduced basis approach to time-dependent equation-of-motion coupled-cluster theory. Physical Review A, 2022, 105, .	2.5	14
117	A study of the valence shell electronic states of pyridazine by photoabsorption spectroscopy and time-dependent density functional theory calculations. Journal of Physics B: Atomic, Molecular and Optical Physics, 2013, 46, 175103.	1.5	13
118	A coupled-cluster study of photodetachment cross sections of closed-shell anions. Journal of Chemical Physics, 2014, 141, 174315.	3.0	13
119	A complex-polarization-propagator protocol for magneto-chiral axial dichroism and birefringence dispersion. Physical Chemistry Chemical Physics, 2016, 18, 13267-13279.	2.8	13
120	State-of-the-art ab initio calculations of the molecular electric quadrupole moments of hydrogen fluoride. Chemical Physics Letters, 2001, 346, 329-333.	2.6	12
121	Density dependence of electric properties of binary mixtures of inert gases. Molecular Physics, 2006, 104, 305-318.	1.7	12
122	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.	1.7	12
123	Spin adapted implementation of EOM-CCSD for triplet excited states: Probing intersystem crossings of acetylacetone at the carbon and oxygen K-edges. Journal of Chemical Physics, 2019, 151, 144107.	3.0	12
124	Lanczos-based equation-of-motion coupled-cluster singles-and-doubles approach to the total photoionization cross section of valence excited states. Journal of Chemical Physics, 2019, 151, 184106.	3.0	12
125	Structure Elucidation of Prenyl- and Geranyl-Substituted Coumarins in Gerbera piloselloides by NMR Spectroscopy, Electronic Circular Dichroism Calculations, and Single Crystal X-ray Crystallography. Molecules, 2020, 25, 1706.	3.8	12
126	Electronic circular dichroism spectra using the algebraic diagrammatic construction schemes of the polarization propagator up to third order. Journal of Chemical Physics, 2021, 154, 064107.	3.0	12

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127	Probing Molecular Chirality of Ground and Electronically Excited States in the UVâ€“vis and X-ray Regimes: An EOM-CCSD Study. Journal of Chemical Theory and Computation, 2022, 18, 1748-1764.	5.3	12
128	MCSCF nuclear magnetic shieldings and spin-rotation constants of 17O in 16O17O16O and 17O16O16O. Chemical Physics Letters, 1998, 287, 677-681.	2.6	11
129	Nitrogen K-Edge X-ray Absorption Spectra of Ammonium and Ammonia in Water Solution: Assessing the Performance of Polarizable Embedding Coupled Cluster Methods. Journal of Physical Chemistry Letters, 2021, 12, 8865-8871.	4.6	11
130	Transient resonant Augerâ€“Meitner spectra of photoexcited thymine. Faraday Discussions, 2021, 228, 555-570.	3.2	11
131	Photoionization Observables from Multi-Reference Dyson Orbitals Coupled to B-Spline DFT and TD-DFT Continuum. Molecules, 2022, 27, 1203.	3.8	11
132	Nonlinear effects in the interaction of time-dependent fields and chiral systems: A computational investigation. Journal of Chemical Physics, 2006, 125, 054107.	3.0	10
133	Identifying the Hamiltonian structure in linear response theory. Journal of Chemical Physics, 2014, 140, 224103.	3.0	10
134	Magnetic circular dichroism spectra from resonant and damped coupled cluster response theory. Journal of Chemical Physics, 2020, 153, 114105.	3.0	10
135	Serrulatane diterpenoids from the leaves of Eremophila glabra and their potential as antihyperglycemic drug leads. Phytochemistry, 2022, 196, 113072.	2.9	10
136	Nuclear spin circular dichroism in fullerenes: a computational study. Chemical Communications, 2014, 50, 15228-15231.	4.1	9
137	The Absorption Spectrum of Guanine Based Radicals: a Comparative Computational Analysis. ChemPhotoChem, 2019, 3, 846-855.	3.0	9
138	Multi-reference approach to the computation of double core-hole spectra. Journal of Chemical Physics, 2021, 155, 131101.	3.0	9
139	Multireference Approach to Normal and Resonant Auger Spectra Based on the One-Center Approximation. Journal of Chemical Theory and Computation, 2022, 18, 4387-4407.	5.3	9
140	Modeling magnetic circular dichroism within the polarizable embedding approach. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	8
141	The Intriguing Case of the Oneâ€Photon and Twoâ€Photon Absorption of a Prototypical Symmetric Squaraine: Comparison of TDDFT and Waveâ€Function Methods. ChemPhotoChem, 2019, 3, 778-793.	3.0	8
142	Taxonomy Driven Discovery of Polyketides from Aspergillus californicus. Journal of Natural Products, 2021, 84, 979-985.	3.0	8
143	Vibrationally resolved coupled-cluster x-ray absorption spectra from vibrational configuration interaction anharmonic calculations. Journal of Chemical Physics, 2020, 153, 234111.	3.0	8
144	Coupled cluster investigation of Sternheimer shieldings and electric field gradient polarizabilities. Journal of Chemical Physics, 2000, 113, 1688-1697.	3.0	7

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145	Density dependence of the electric-field-gradient induced birefringence of the helium, neon and argon gases. Molecular Physics, 2003, 101, 1851-1865.	1.7	7
146	Optically induced circular and axial birefringences in achiral fluids: anab initiostudy of the optical Faraday effect. Molecular Physics, 2006, 104, 2173-2192.	1.7	7
147	Synthesis, characterization and assignment of the absolute configuration of 4,4-dimethyl-5-oxo-tetrahydrofuran-3-carboxylic acid and its esters: a combined experimental and theoretical investigation. Tetrahedron: Asymmetry, 2009, 20, 1459-1467.	1.8	7
148	On the Absolute Configuration of Chiral 1,4-Dihydropyridazines Synthesized by Organocatalysed Reactions. Journal of Organic Chemistry, 2013, 78, 11670-11679.	3.2	7
149	Magnetic Circular Dichroism of Naphthalene Derivatives: A Coupled Cluster Singles and Approximate Doubles and Time-Dependent Density Functional Theory Study. Journal of Physical Chemistry A, 2021, 125, 243-250.	2.5	7
150	Excited state absorption of DNA bases in the gas phase and in chloroform solution: a comparative quantum mechanical study. Physical Chemistry Chemical Physics, 2022, 24, 4987-5000.	2.8	7
151	Multi-electron excitation contributions towards primary and satellite states in the photoelectron spectrum. Physical Chemistry Chemical Physics, 2022, 24, 8329-8343.	2.8	7
152	Efficient implementation of molecular CCSD gradients with Cholesky-decomposed electron repulsion integrals. Journal of Chemical Physics, 2022, 156, .	3.0	7
153	Orbital nonrelaxed coupled cluster singles and doubles with perturbative triples corrections calculations of first-order one-electron properties. Journal of Chemical Physics, 2002, 117, 9983-9990.	3.0	6
154	Investigation of electric-field-gradient-induced birefringence in H2 and D2. Theoretical Chemistry Accounts, 2007, 117, 969-977.	1.4	6
155	Circular and linear magnetic birefringences in xenon at Î» = 1064 nm. Journal of Chemical Physics, 2015, 142, 124313.	3.0	6
156	Zeeman effect in sulfur monoxide. Astronomy and Astrophysics, 2017, 605, A20.	5.1	6
157	Relation between molecular electronic structure and nuclear spin-induced circular dichroism. Scientific Reports, 2017, 7, 46617.	3.3	6
158	Damped (linear) response theory within the resolution-of-identity coupled cluster singles and approximate doubles (RI-CC2) method. Journal of Chemical Physics, 2021, 154, 124110.	3.0	6
159	MCSCF calculations of hypermagnetizabilities and nuclear shielding polarizabilities of CO and CH4. Molecular Physics, 1996, 88, 931-948.	1.7	6
160	NEXAFS and MS-AES spectroscopy of the C 1s and Cl 2p excitation and ionization of chlorobenzene: Production of dicationic species. Physical Chemistry Chemical Physics, 2021, 23, 27484-27497.	2.8	6
161	On the origin independence of the Verdet tensor^{â€}. Molecular Physics, 2013, 111, 1405-1413.	1.7	5
162	Molecular Photoionization and Photodetachment Cross Sections Based on L^{2} Basis Sets: Theory and Selected Examples. Progress in Theoretical Chemistry and Physics, 2021, , 151-179.	0.2	5

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163	Inner-shell photoabsorption and photoionisation cross-sections of valence excited states from asymmetric-Lanczos equation-of-motion coupled cluster singles and doubles theory. Molecular Physics, 2021, 119, .	1.7	5
164	Gauge-origin-independent magnetizabilities of solvated molecules using the polarizable continuum model. Journal of Chemical Physics, 2005, 123, 204104.	3.0	4
165	A study of the valence shell electronic states of s-triazine by photoabsorption spectroscopy and ab initio calculations. Chemical Physics, 2016, 477, 96-104.	1.9	4
166	One-Photon Absorption Properties from a Hybrid Polarizable Density Embedding/Complex Polarization Propagator Approach for Polarizable Solutions. Journal of Chemical Theory and Computation, 2018, 14, 2145-2154.	5.3	4
167	Insights on the site-selective fragmentation of CF2Cl2 and CH2Cl2 at the chlorine K-edge from ab initio calculations. Chemical Physics, 2021, 548, 111226.	1.9	4
168	Molecular Dipole Moments within the Incremental Scheme Using the Domain-Specific Basis-Set Approach. Journal of Chemical Theory and Computation, 2016, 12, 3040-3052.	5.3	3
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