Dage Sundholm

List of Publications by Year
in descending order

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207	8,922	36303	60623
papers	citations	51 h-index	81 g-index

211	211	211	5062
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Calculation of current densities using gauge-including atomic orbitals. Journal of Chemical Physics, 2004, 121, 3952-3963.	3.0	393
2	The gauge including magnetically induced current method. Physical Chemistry Chemical Physics, 2011, 13, 20500.	2.8	326
3	Au32: A 24-Carat Golden Fullerene. Angewandte Chemie - International Edition, 2004, 43, 2678-2681.	13.8	285
4	Calculations of magnetically induced current densities: theory and applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 639-678.	14.6	244
5	Fully numerical hartree-fock methods for molecules. Computer Physics Reports, 1986, 4, 313-344.	2.2	240
6	Ab initio determination of the induced ring current in aromatic molecules. Physical Chemistry Chemical Physics, 1999, 1, 3429-3435.	2.8	173
7	Density functional theory calculations of the visible spectrum of chlorophyll a. Chemical Physics Letters, 1999, 302, 480-484.	2.6	170
8	Rovibrationally averaged nuclear magnetic shielding tensors calculated at the coupledâ€cluster level. Journal of Chemical Physics, 1996, 105, 11051-11059.	3.0	169
9	Magnetically Induced Current Densities in Aromatic, Antiaromatic, Homoaromatic, and Nonaromatic Hydrocarbons. Journal of Physical Chemistry A, 2009, 113, 8668-8676.	2.5	164
10	Luminescent Characterization of Solution Oligomerization Process Mediated Goldâ^'Gold Interactions. DFT Calculations on [Au2Ag2R4L2]nMoieties. Journal of the American Chemical Society, 2000, 122, 7287-7293.	13.7	140
11	A numerical Hartree-Fock program for diatomic molecules. Computer Physics Communications, 1996, 98, 346-358.	7.5	123
12	Two-dimensional, fully numerical molecular calculations. Molecular Physics, 1985, 56, 1411-1418.	1.7	113
13	Sphere Currents of Buckminsterfullerene. Angewandte Chemie - International Edition, 2005, 44, 1843-1846.	13.8	113
14	Interpretation of the electronic absorption spectrum of free-base porphin using time-dependent density-functional theory. Physical Chemistry Chemical Physics, 2000, 2, 2275-2281.	2.8	109
15	Calculation of spin-current densities using gauge-including atomic orbitals. Journal of Chemical Physics, 2011, 134, 054123.	3.0	109
16	Magnetic-Shielding Calculations on Al42-and Analogues. A New Family of Aromatic Molecules?. Journal of Physical Chemistry A, 2001, 105, 9939-9944.	2.5	103
17	Cyclo[18]carbon: Insight into Electronic Structure, Aromaticity, and Surface Coupling. Journal of Physical Chemistry Letters, 2019, 10, 6701-6705.	4.6	103
18	The aromatic pathways of porphins, chlorins and bacteriochlorins. Physical Chemistry Chemical Physics, 2000, 2, 2145-2151.	2.8	99

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19	Properties of WAu12. Physical Chemistry Chemical Physics, 2004, 6, 11-22.	2.8	97
20	Comparison of the electronic excitation spectra of chlorophyll a and pheophytin a calculated at density functional theory level. Chemical Physics Letters, 2000, 317, 545-552.	2.6	87
21	Magnetically induced current densities in Al42â˜ and Al44â˜ species studied at the coupled-cluster level. Journal of Chemical Physics, 2005, 122, 214308.	3.0	87
22	Two-dimensional fully numerical solutions of molecular SchrÃ¶dinger equations. I. One-electron molecules. International Journal of Quantum Chemistry, 1983, 23, 309-317.	2.0	84
23	The Aromatic Character of Magnesium Porphyrins. Journal of Organic Chemistry, 2000, 65, 5233-5237.	3.2	83
24	Aromatic Pathways of Porphins, Chlorins, and Bacteriochlorins. Journal of Organic Chemistry, 2012, 77, 3408-3414.	3.2	80
25	Nuclear quadrupole moment of lithium from combined fully numerical and discrete basis-set calculations on LiH. Chemical Physics Letters, 1984, 112, 1-9.	2.6	79
26	Two-Dimensional fully numerical solutions of molecular SchrÃ¶dinger equations. II. Solution of the Poisson equation and results for singlet states of H2and HeH+. International Journal of Quantum Chemistry, 1983, 23, 319-323.	2.0	78
27	Electric quadrupole moment of the 27Al nucleus: Converging results from the AlF and AlCl molecules and the Al atom. Chemical Physics Letters, 1999, 304, 414-422.	2.6	73
28	Energetics and dynamics of a light-driven sodium-pumping rhodopsin. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 7043-7048.	7.1	73
29	â€˜â€˜Atomicâ€™â€™ determination of theNa23,Mg25, andAl27nuclear quadrupole moments: How accurate are the â€˜â€˜muonicâ€™â€™ values?. Physical Review Letters, 1992, 68, 927-930.	7.8	72
30	Experimental and Computational Studies of Alkali-Metal Coinage-Metal Clusters. Journal of Physical Chemistry A, 2006, 110, 4244-4250.	2.5	70
31	Benchmarking the Performance of Time-Dependent Density Functional Theory Methods on Biochromophores. Journal of Chemical Theory and Computation, 2020, 16, 587-600.	5.3	69
32	Large multiconfiguration Hartreeâ€“Fock calculations on the hyperfine structure of B(2P) and the nuclear quadrupole moments of10B and11B. Journal of Chemical Physics, 1991, 94, 5051-5055.	3.0	65
33	Aromatic Pathways in Twisted Hexaphyrins. Journal of Physical Chemistry A, 2010, 114, 7153-7161.	2.5	65
34	Large multiconfigurational Hartree-Fock calculations on the hyperfine structure of Li(2S) and Li(2P). Physical Review A, 1990, 42, 2614-2621.	2.5	64
35	The Spin Distribution in Low-Spin Iron Porphyrins. Journal of the American Chemical Society, 2002, 124, 11771-11780.	13.7	64
36	Stairway to the Conical Intersection:Â A Computational Study of the Retinal Isomerization. Journal of Physical Chemistry A, 2007, 111, 8766-8773.	2.5	63

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37	Finite element multiconfiguration Hartree-Fock calculations on carbon, oxygen, and neon: the nuclear quadrupole moments of carbon-11, oxygen-17, and neon-21. The Journal of Physical Chemistry, 1992, 96, 627-630.	2.9	62
38	The nuclear quadrupole moment of 14N obtained from finite-element MCHF calculationson N2+ (2p;) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	2.6	61
39	The aromaticity and antiaromaticity of dehydroannulenes. Physical Chemistry Chemical Physics, 2001, 3, 2433-2437.	2.8	61
40	Analysis of the magnetically induced current density of molecules consisting of annelated aromatic and antiaromatic hydrocarbon rings. Physical Chemistry Chemical Physics, 2016, 18, 15934-15942.	2.8	61
41	Two-Dimensional, fully numerical molecular calculations. IV. hartree-fock-slater results on second-row diatomic molecules. International Journal of Quantum Chemistry, 1985, 27, 601-612.	2.0	59
42	Beryllium atom reinvestigated: A comparison between theory and experiment. Physical Review A, 1991, 43, 3355-3364.	2.5	59
43	Two-dimensional fully numerical solutions of molecular Hartree-Fock equations: LiH and BH. Chemical Physics Letters, 1983, 96, 1-3.	2.6	58
44	Large MCHF calculations on the hyperfine structure of Be(3PO): the nuclear quadrupole moment of 9Be. Chemical Physics Letters, 1991, 177, 91-97.	2.6	57
45	Effect of Fluorine Substitution on the Aromaticity of Polycyclic Hydrocarbons. Journal of Physical Chemistry A, 2012, 116, 10257-10268.	2.5	57
46	Proteinâ€Induced Color Shift of Carotenoids in Î²â€Crustacyanin. Angewandte Chemie - International Edition, 2015, 54, 11564-11566.	13.8	57
47	Magnetically Induced Currents in [n]Cycloparaphenylenes, n = 6â^11. Journal of Organic Chemistry, 2010, 75, 5867-5874.	3.2	56
48	Computational studies of photophysical properties of porphin, tetraphenylporphyrin and tetrabenzoporphyrin. Physical Chemistry Chemical Physics, 2012, 14, 11508.	2.8	56
49	Reduction of the virtual space for coupled-cluster excitation energies of large molecules and embedded systems. Journal of Chemical Physics, 2011, 134, 214114.	3.0	55
50	Calculation of absorption and emission spectra of [n]cycloparaphenylenes: the reason for the large Stokes shift. Physical Chemistry Chemical Physics, 2010, 12, 2751.	2.8	53
51	Nuclear quadrupole moment of nitrogen from combined fully numerical and discrete basis-set calculations on NO+ and N2. Chemical Physics, 1986, 101, 219-225.	1.9	52
52	Finite element multiconfiguration Hartreeâ€“Fock determination of the nuclear quadrupole moments of chlorine, potassium, and calcium isotopes. Journal of Chemical Physics, 1993, 98, 7152-7158.	3.0	49
53	Change in electron and spin density upon electron transfer to haem. Biochimica Et Biophysica Acta - Bioenergetics, 2002, 1553, 183-187.	1.0	49
54	Polycyclic antiaromatic hydrocarbons. Physical Chemistry Chemical Physics, 2008, 10, 6630.	2.8	49

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55	Isotope and temperature effects on nuclear magnetic shieldings and spin-rotation constants calculated at the coupled-cluster level. Molecular Physics, 1997, 92, 1007-1014.	1.7	47
56	The chemistry of the CuB site in cytochrome c oxidase and the importance of its unique Hisâ€“Tyr bond. Biochimica Et Biophysica Acta - Bioenergetics, 2009, 1787, 221-233.	1.0	47
57	Electrostatic spectral tuning mechanism of the green fluorescent protein. Physical Chemistry Chemical Physics, 2013, 15, 4491.	2.8	47
58	Calculation of vibrationally resolved absorption spectra of acenes and pyrene. Physical Chemistry Chemical Physics, 2019, 21, 21094-21103.	2.8	47
59	Coupled-cluster calculations of spin-rotation constants. Molecular Physics, 1997, 91, 449-458.	1.7	46
60	Nuclear quadrupole moments of bromine and iodine from combined atomic and molecular data. Physical Review A, 2001, 64, .	2.5	46
61	Coupled-cluster studies of the lowest excited states of the 11-cis-retinal chromophore. Physical Chemistry Chemical Physics, 2007, 9, 2862.	2.8	46
62	Two-dimensional, fully numerical molecular calculations. Molecular Physics, 1987, 60, 597-604.	1.7	45
63	Coupled-cluster and density functional theory studies of the electronic excitation spectra of trans-1,3-butadiene and trans-2-propeniminium. Journal of Chemical Physics, 2009, 131, 024301.	3.0	44
64	Gauge-Origin Independent Calculations of the Anisotropy of the Magnetically Induced Current Densities. Journal of Physical Chemistry A, 2016, 120, 5658-5664.	2.5	44
65	The Effect of Protein Environment on Photoexcitation Properties of Retinal. Journal of Physical Chemistry B, 2012, 116, 2249-2258.	2.6	43
66	Spectral Tuning of Rhodopsin and Visual Cone Pigments. Journal of the American Chemical Society, 2014, 136, 2723-2726.	13.7	43
67	Calculations of current densities for neutral and doubly charged persubstituted benzenes using effective core potentials. Physical Chemistry Chemical Physics, 2017, 19, 7124-7131.	2.8	43
68	Benchmarking Magnetizabilities with Recent Density Functionals. Journal of Chemical Theory and Computation, 2021, 17, 1457-1468.	5.3	43
69	Two-dimensional, fully numerical solutions of second-order Dirac equations for diatomic molecules. part 3. Physica Scripta, 1987, 36, 400-402.	2.5	42
70	Aromatic pathways in mono- and bisphosphorous singly MÃ¶bius twisted [28] and [30]hexaphyrins. Physical Chemistry Chemical Physics, 2011, 13, 20659.	2.8	41
71	Computational Studies of Aromatic and Photophysical Properties of Expanded Porphyrins. Journal of Physical Chemistry A, 2018, 122, 4756-4767.	2.5	41
72	A density-functional-theory study of bacteriochlorophyll b. Physical Chemistry Chemical Physics, 2003, 5, 4265.	2.8	40

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73	Benchmarking the Approximate Second-Order Coupled-Cluster Method on Biochromophores. Journal of Chemical Theory and Computation, 2011, 7, 2473-2484.	5.3	40
74	Closed-shell paramagnetic porphyrinoids. Chemical Communications, 2017, 53, 9866-9869.	4.1	40
75	The exactness of the extended Koopmansâ€™ theorem: A numerical study. Journal of Chemical Physics, 1993, 98, 3999-4002.	3.0	39
76	Current density and molecular magnetic properties. Chemical Communications, 2021, 57, 12362-12378.	4.1	39
77	Large MCHF calculations on the electron affinity of boron. Chemical Physics Letters, 1990, 171, 53-57.	2.6	38
78	A modified variation-perturbation approach to zero-point vibrational motion. Theoretical Chemistry Accounts, 2000, 103, 365-373.	1.4	38
79	The Role of the Î²-Ionone Ring in the Photochemical Reaction of Rhodopsin. Journal of Physical Chemistry A, 2007, 111, 27-33.	2.5	38
80	Insights into Magnetically Induced Current Pathways and Optical Properties of Isophlorins. Journal of Physical Chemistry A, 2013, 117, 9062-9068.	2.5	38
81	Calculating rate constants for intersystem crossing and internal conversion in the Franckâ€“Condon and Herzbergâ€“Teller approximations. Physical Chemistry Chemical Physics, 2019, 21, 18495-18500.	2.8	38
82	Spin and charge distribution in iron porphyrin models: A coupled cluster and density-functional study. Journal of Chemical Physics, 2004, 120, 3229-3236.	3.0	37
83	Computational studies of semiconductor quantum dots. Physical Chemistry Chemical Physics, 2008, 10, 4535.	2.8	37
84	Exploring the Stability of Golden Fullerenes. Journal of Physical Chemistry C, 2008, 112, 19311-19315.	3.1	37
85	Relation Between Ring Currents and Hydrogenation Enthalpies for Assessing the Degree of Aromaticity. Journal of Physical Chemistry A, 2017, 121, 7282-7289.	2.5	37
86	Magnetically Induced Currents in Bianthraquinodimethane-Stabilized MÃ¶bius and HÃ¼ckel [16]Annulenes. Journal of Organic Chemistry, 2009, 74, 6495-6502.	3.2	36
87	Excited State Potential Energy Surfaces of Polyenes and Protonated Schiff Bases. Journal of Chemical Theory and Computation, 2009, 5, 2401-2414.	5.3	36
88	Nuclear quadrupole moments ofS33andS35. Physical Review A, 1990, 42, 1160-1164.	2.5	35
89	Hydrogen-bond strengths by magnetically induced currents. Physical Chemistry Chemical Physics, 2011, 13, 434-437.	2.8	35
90	Importance of Vibronic Effects in the UVâ€“Vis Spectrum of the 7,7,8,8-Tetracyanoquinodimethane Anion. Journal of Chemical Theory and Computation, 2016, 12, 5058-5066.	5.3	35

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91	Density-functional studies of excited states of silicon nanoclusters. Physical Review B, 2005, 72, .	3.2	34
92	Aromaticity of the doubly charged [8]circulenes. Physical Chemistry Chemical Physics, 2016, 18, 8980-8992.	2.8	34
93	Calculation of Magnetically Induced Currents in Hydrocarbon Nanorings. Journal of Physical Chemistry A, 2008, 112, 13584-13592.	2.5	33
94	C72: gaudiene, a hollow and aromatic all-carbon molecule. Physical Chemistry Chemical Physics, 2013, 15, 9025.	2.8	33
95	Exploring the Light-Capturing Properties of Photosynthetic Chlorophyll Clusters Using Large-Scale Correlated Calculations. Journal of Chemical Theory and Computation, 2016, 12, 2644-2651.	5.3	32
96	Towards an accurate determination of the nuclear quadrupole moment of Li from molecular data: LiF. Chemical Physics Letters, 1988, 143, 163-168.	2.6	31
97	Tetraberyllium-Î·⁴-oxo-hexa(arylcarboxylates). Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2001, 56, 979-989.	0.7	31
98	Computational studies of 13C NMR chemical shifts of saccharides. Physical Chemistry Chemical Physics, 2005, 7, 2561.	2.8	31
99	Dynamics and magnetic resonance properties of Sc3C2@C80 and its monoanion. Physical Chemistry Chemical Physics, 2008, 10, 7158.	2.8	31
100	Two-dimensional fully numerical MC SCF calculations on H2 and LiH: The dipole moment of LiH. Chemical Physics Letters, 1984, 105, 573-576.	2.6	30
101	Finite-element multiconfiguration Hartree-Fock calculations of the atomic quadrupole moments of excited states of Be, Al, In, Ne, Ar, Kr, and Xe. Physical Review A, 1993, 47, 2672-2679.	2.5	30
102	Coupled-Cluster Studies of Extensive Green Fluorescent Protein Models Using the Reduced Virtual Space Approach. Journal of Physical Chemistry B, 2015, 119, 2933-2945.	2.6	30
103	Aromaticity of Even-Number Cyclo[n]carbons (n = 6â€“100). Journal of Physical Chemistry A, 2020, 124, 10849-10855.	2.5	30
104	The electron correlation contribution to the nuclear magnetic shielding tensor of the hydrogen molecule. Chemical Physics Letters, 1995, 243, 264-268.	2.6	29
105	Aromatic pathways in thieno-bridged porphyrins: understanding the influence of the direction of the thiophene ring on the aromatic character. Molecular Physics, 2013, 111, 1364-1372.	1.7	29
106	Electronic and optical properties of metalloporphyrins of zinc on TiO₂ cluster in dye-sensitized solar-cells (DSSC). A quantum chemistry study. RSC Advances, 2017, 7, 42677-42684.	3.6	29
107	Two-dimensional, fully numerical molecular calculations. Molecular Physics, 1985, 55, 627-635.	1.7	28
108	New insights into aromatic pathways of carbachlorins and carbaporphyrins based on calculations of magnetically induced current densities. Physical Chemistry Chemical Physics, 2016, 18, 11932-11941.	2.8	28

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109	Theoretical studies as a tool for understanding the aromatic character of porphyrinoid compounds. Chemical Modelling, 0, , 1-42.	0.4	28
110	On perturbation expansions of the extended Koopmans' theorem. Chemical Physics Letters, 1998, 288, 282-288.	2.6	27
111	Density functional studies of the luminescence of Si29H36. Physical Chemistry Chemical Physics, 2004, 6, 2044.	2.8	27
112	Parallel implementation of a direct method for calculating electrostatic potentials. Journal of Chemical Physics, 2007, 126, 094101.	3.0	27
113	Predicting the degree of aromaticity of novel carbaporphyrinoids. Physical Chemistry Chemical Physics, 2015, 17, 14215-14222.	2.8	27
114	Novel hollow all-carbon structures. Nanoscale, 2015, 7, 15886-15894.	5.6	27
115	Coreâ€"valence correlation effects on the ground state electron affinity of calcium. Chemical Physics Letters, 1994, 217, 451-455.	2.6	26
116	On the Aromaticity of the Planar Hydrogen-Bonded (HF)3Trimer. Journal of Chemical Theory and Computation, 2006, 2, 761-764.	5.3	26
117	The aromatic character of thienopyrrole-modified 20Ï€-electron porphyrinoids. Physical Chemistry Chemical Physics, 2014, 16, 11010.	2.8	26
118	[Hg 4 Te 8 (Te 2) 4] 8â˜ : A Heavy Metal Porphyrinoid Embedded in a Lamellar Structure. Angewandte Chemie - International Edition, 2018, 57, 8770-8774.	13.8	26
119	Two-dimensional, fully numerical solution of the molecular Dirac equation. Dirac-Slater calculations on LiH, Li2, BH and CH+. Chemical Physics Letters, 1988, 149, 251-256.	2.6	24
120	First Principles Calculations of the Absorption Spectrum of Si29H36. Nano Letters, 2003, 3, 847-849.	9.1	23
121	Real-space numerical grid methods in quantum chemistry. Physical Chemistry Chemical Physics, 2015, 17, 31357-31359.	2.8	23
122	Aromatic Pathways in Carbathiaporphyrins. Journal of Physical Chemistry A, 2015, 119, 1201-1207.	2.5	23
123	Antiaromatic Character of 16 Ï€ Electron Octaethylporphyrins: Magnetically Induced Ring Currents from DFT-GIMIC Calculations. Journal of Physical Chemistry A, 2015, 119, 2344-2350.	2.5	23
124	Non-intersecting ring currents in [12]infinitene. Physical Chemistry Chemical Physics, 2022, 24, 6404-6409.	2.8	23
125	Calculation of ring-current susceptibilities for potentially homoaromatic hydrocarbons. Computational and Theoretical Chemistry, 2003, 633, 123-136.	1.5	21
126	Bicycloaromaticity and Baird-type bicycloaromaticity of dithienothiophene-bridged [34]octaphyrins. Physical Chemistry Chemical Physics, 2018, 20, 17705-17713.	2.8	21

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127	Nuclear quadrupole moments of gallium isotopes obtained from finite-element MCHF calculations on the 4p2P3/2 state of Ga. Chemical Physics Letters, 1998, 291, 414-418.	2.6	20
128	Ab Initio Studies of Triplet-State Properties for Organic Semiconductor Molecules. Journal of Physical Chemistry C, 2012, 116, 15203-15217.	3.1	20
129	Magnetically Induced Current Densities in Toroidal Carbon Nanotubes. Journal of Physical Chemistry C, 2019, 123, 15354-15365.	3.1	20
130	Aromatic pathways in conjugated rings connected by single bonds. International Journal of Quantum Chemistry, 2011, 111, 848-857.	2.0	19
131	Optical and magnetic properties of antiaromatic porphyrinoids. Physical Chemistry Chemical Physics, 2017, 19, 25979-25988.	2.8	19
132	Magnetically Induced Ring-Current Strengths in MÃ¶bius Twisted Annulenes. Journal of Physical Chemistry Letters, 2018, 9, 1627-1632.	4.6	19
133	Finite-element multiconfiguration Hartree-Fock calculations of the atomic quadrupole moments ofC+(2P) andNe+(2P). Physical Review A, 1994, 49, 3453-3456.	2.5	18
134	Optical properties of sila-adamantane nanoclusters from density-functional theory. Physical Review B, 2006, 74, .	3.2	18
135	Calculations of current densities and aromatic pathways in cyclic porphyrin and isoporphyrin arrays. Physical Chemistry Chemical Physics, 2017, 19, 12794-12803.	2.8	18
136	Aromatic and Antiaromatic Pathways in Triphyrin(2.1.1) Annelated with Benzo[b]heterocycles. Chemistry - A European Journal, 2019, 25, 15477-15482.	3.3	18
137	When are Antiaromatic Molecules Paramagnetic?. Journal of Physical Chemistry C, 2020, 124, 21027-21035.	3.1	18
138	Multiconfiguration selfâ€consistent field quadratic response calculations of the twoâ€photon transition probability rate constants for argon. Journal of Chemical Physics, 1994, 101, 4931-4935.	3.0	17
139	Fully numerical soluti ons of molecular Dirac equations for highly charged one-electron homonuclear diatomic molecules. Chemical Physics Letters, 1994, 223, 469-473.	2.6	17
140	Ab initiocalculations of the ground-state electron affinities of gallium and indium. Journal of Physics B: Atomic, Molecular and Optical Physics, 1999, 32, 5853-5859.	1.5	17
141	Tuning the Proteinâ€Induced Absorption Shifts of Retinal in Engineered Rhodopsin Mimics. Chemistry - A European Journal, 2016, 22, 8254-8261.	3.3	17
142	Interplay of Aromaticity and Antiaromaticity in N-Doped Nanographenes. Journal of Physical Chemistry A, 2020, 124, 695-703.	2.5	17
143	Spatial Contributions to Nuclear Magnetic Shieldings. Journal of Physical Chemistry A, 2021, 125, 1778-1786.	2.5	17
144	Magnetically Induced Ring-Current Strengths of Planar and Nonplanar Molecules: New Insights from the Pseudo-Ï€ Model. Journal of Physical Chemistry A, 2021, 125, 5753-5764.	2.5	17

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145	A Photoelectron Spectroscopic and Computational Study of Sodium Auride Clusters, NanAun-(n= 1â^'3). Journal of Physical Chemistry A, 2007, 111, 7555-7561.	2.5	16
146	Absorption shifts of diastereotopically ligated chlorophyll dimers of photosystem I. Physical Chemistry Chemical Physics, 2019, 21, 6851-6858.	2.8	16
147	A multiconfiguration selfâ€consistentâ€field response study of oneâ€and twoâ€photon dipole transitions between the Xâ€‰1Î£+ and Aâ€‰1Î states of CO. Journal of Chemical Physics, 1995, 102, 4143-4150.	3.0	15
148	Coupled-cluster studies of the electronic excitation spectra of silanes. Journal of Chemical Physics, 2006, 125, 144314.	3.0	15
149	The molecular structure of a curl-shaped retinal isomer. Journal of Molecular Modeling, 2008, 14, 717-726.	1.8	15
150	Evaluating Shieldingâ€Based Ringâ€Current Models by Using the Gaugeâ€Including Magnetically Induced Current Method. Journal of the Chinese Chemical Society, 2016, 63, 93-100.	1.4	15
151	The influence of heteroatoms on the aromatic character and the current pathways of B₂N₂-dibenzo[a,e]pentalenes. Physical Chemistry Chemical Physics, 2017, 19, 20213-20223.	2.8	15
152	Perhalophenyl Three-Coordinate Gold(I) Complexes as TADF Emitters: A Photophysical Study from Experimental and Computational Viewpoints. Inorganic Chemistry, 2020, 59, 14236-14244.	4.0	15
153	Integration of global ring currents using the AmpÃ¨reâ€“Maxwell law. Physical Chemistry Chemical Physics, 2022, 24, 624-628.	2.8	15
154	The aromatic character of [10]annulenes and dicupra[10]annulenes from current density calculations. Physical Chemistry Chemical Physics, 2018, 20, 1337-1346.	2.8	14
155	Response to â€˜â€˜Comment on â€˜The exactness of the extended Koopmansâ€™ theorem: A numerical studyâ€™â€™ [J. Chem. Phys. 99, 6221 (1993)]. Journal of Chemical Physics, 1993, 99, 6222-6223.	3.0	13
156	The grid-based fast multipole method â€“ a massively parallel numerical scheme for calculating two-electron interaction energies. Physical Chemistry Chemical Physics, 2015, 17, 31480-31490.	2.8	13
157	Insights into Molecular Structures and Optical Properties of Stacked [Au₃(RNâ•CRâ€²)₃]_n Complexes. Inorganic Chemistry, 2018, 57, 718-730.	4.0	13
158	Calculation of vibrationally resolved absorption and fluorescence spectra of the rylenes. Physical Chemistry Chemical Physics, 2020, 22, 2379-2385.	2.8	13
159	Core-electron contributions to the molecular magnetic response. Physical Chemistry Chemical Physics, 2022, 24, 12158-12166.	2.8	13
160	Finiteâ€element multiconfiguration Hartreeâ€“Fock calculations on the excitation energies and the ionization potential of oxygen. Journal of Chemical Physics, 1992, 96, 5229-5232.	3.0	12
161	Finite element multiconfiguration Hartree-Fock determination of the atomic quadrupole moment of Ca(3d4s; 1D). Chemical Physics Letters, 1992, 198, 526-530.	2.6	12
162	Nuclear Magnetic Shieldings of Stacked Aromatic and Antiaromatic Molecules. Journal of Chemical Theory and Computation, 2017, 13, 1952-1962.	5.3	12

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163	An Ab Initio Study of Structure and Energetics of Free-Base Bonellin-Dimethylester Isomers and Transition States. Chemistry - A European Journal, 1999, 5, 267-273.	3.3	11
164	Theoretical investigation of photoelectron spectra and magnetically induced current densities in ring-shaped transition-metal oxides. Theoretical Chemistry Accounts, 2011, 129, 701-713.	1.4	11
165	Construction of the Fock Matrix on a Grid-Based Molecular Orbital Basis Using GPGPUs. Journal of Chemical Theory and Computation, 2015, 11, 2053-2062.	5.3	11
166	A block preconditioned conjugate gradient method for solving high-order finite element matrix equations. Computer Physics Communications, 1988, 49, 409-415.	7.5	10
167	The nuclear quadrupole moment of 14N obtained from finite element MCHF calculations on N+ (2p3p) 1P. Chemical Physics Letters, 1994, 226, 17-21.	2.6	10
168	Bright luminescence from silane substituted and bridged silicon nanoclusters. Physical Chemistry Chemical Physics, 2006, 8, 4228.	2.8	10
169	Calculation of magnetic response properties of tetrazines. RSC Advances, 2020, 10, 18124-18130.	3.6	10
170	A Generalized Grid-Based Fast Multipole Method for Integrating Helmholtz Kernels. Journal of Chemical Theory and Computation, 2017, 13, 654-665.	5.3	9
171	[Hg 4 Te 8 (Te 2) 4] 8â˜ : ein Schwermetallâ€Porphyrinoid in einer lamellaren Struktur. Angewandte Chemie, 2018, 130, 8906-8910.	2.0	9
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