

Dage Matts BÄrje Sundholm

List of Publications by Year in descending order

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176
papers

6,637
citations

71061

41
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73
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181
all docs

181
docs citations

181
times ranked

4111
citing authors

#	ARTICLE	IF	CITATIONS
1	Calculation of current densities using gauge-including atomic orbitals. <i>Journal of Chemical Physics</i> , 2004, 121, 3952-3963.	1.2	393
2	The gauge including magnetically induced current method. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20500.	1.3	326
3	Au ₃₂ : A 24-Carat Golden Fullerene. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 2678-2681.	7.2	285
4	Calculations of magnetically induced current densities: theory and applications. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2016, 6, 639-678.	6.2	244
5	Fully numerical hartree-fock methods for molecules. <i>Computer Physics Reports</i> , 1986, 4, 313-344.	2.3	240
6	Ab initio determination of the induced ring current in aromatic molecules. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 3429-3435.	1.3	173
7	Magnetically Induced Current Densities in Aromatic, Antiaromatic, Homoaromatic, and Nonaromatic Hydrocarbons. <i>Journal of Physical Chemistry A</i> , 2009, 113, 8668-8676.	1.1	164
8	Luminescent Characterization of Solution Oligomerization Process Mediated Gold-Gold Interactions. DFT Calculations on [Au ₂ Ag ₂ R ₄ L ₂] _n Moieties. <i>Journal of the American Chemical Society</i> , 2000, 122, 7287-7293.	6.6	140
9	A numerical Hartree-Fock program for diatomic molecules. <i>Computer Physics Communications</i> , 1996, 98, 346-358.	3.0	123
10	Two-dimensional, fully numerical molecular calculations. <i>Molecular Physics</i> , 1985, 56, 1411-1418.	0.8	113
11	Sphere Currents of Buckminsterfullerene. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 1843-1846.	7.2	113
12	Interpretation of the electronic absorption spectrum of free-base porphyrin using time-dependent density-functional theory. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 2275-2281.	1.3	109
13	Calculation of spin-current densities using gauge-including atomic orbitals. <i>Journal of Chemical Physics</i> , 2011, 134, 054123.	1.2	109
14	Cyclo[18]carbon: Insight into Electronic Structure, Aromaticity, and Surface Coupling. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 6701-6705.	2.1	103
15	The aromatic pathways of porphyrins, chlorins and bacteriochlorins. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 2145-2151.	1.3	99
16	Properties of WAu ₁₂ . <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 11-22.	1.3	97
17	The Aromatic Character of Magnesium Porphyrins. <i>Journal of Organic Chemistry</i> , 2000, 65, 5233-5237.	1.7	83
18	Aromatic Pathways of Porphyrins, Chlorins, and Bacteriochlorins. <i>Journal of Organic Chemistry</i> , 2012, 77, 3408-3414.	1.7	80

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19	First-principles method for calculating the rate constants of internal-conversion and intersystem-crossing transitions. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 6121-6133.	1.3	79
20	Energetics and dynamics of a light-driven sodium-pumping rhodopsin. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 7043-7048.	3.3	73
21	Benchmarking the Performance of Time-Dependent Density Functional Theory Methods on Biochromophores. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 587-600.	2.3	69
22	Large multiconfiguration Hartree-Fock calculations on the hyperfine structure of B(2P) and the nuclear quadrupole moments of 10B and 11B. <i>Journal of Chemical Physics</i> , 1991, 94, 5051-5055.	1.2	65
23	Aromatic Pathways in Twisted Hexaphyrins. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7153-7161.	1.1	65
24	Large multiconfigurational Hartree-Fock calculations on the hyperfine structure of Li(2S) and Li(2P). <i>Physical Review A</i> , 1990, 42, 2614-2621.	1.0	64
25	The aromaticity and antiaromaticity of dehydroannulenes. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 2433-2437.	1.3	61
26	Analysis of the magnetically induced current density of molecules consisting of annelated aromatic and antiaromatic hydrocarbon rings. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 15934-15942.	1.3	61
27	Effect of Fluorine Substitution on the Aromaticity of Polycyclic Hydrocarbons. <i>Journal of Physical Chemistry A</i> , 2012, 116, 10257-10268.	1.1	57
28	Protein-Induced Color Shift of Carotenoids in β -Crustacyanin. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 11564-11566.	7.2	57
29	Magnetically Induced Currents in [n]Cycloparaphenylenes, $\langle i \rangle_n \langle i \rangle = 6n^{11}$. <i>Journal of Organic Chemistry</i> , 2010, 75, 5867-5874.	1.7	56
30	Computational studies of photophysical properties of porphin, tetraphenylporphyrin and tetrabenzoporphyrin. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 11508.	1.3	56
31	Reduction of the virtual space for coupled-cluster excitation energies of large molecules and embedded systems. <i>Journal of Chemical Physics</i> , 2011, 134, 214114.	1.2	55
32	Calculation of absorption and emission spectra of [n]cycloparaphenylenes: the reason for the large Stokes shift. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 2751.	1.3	53
33	Finite element multiconfiguration Hartree-Fock determination of the nuclear quadrupole moments of chlorine, potassium, and calcium isotopes. <i>Journal of Chemical Physics</i> , 1993, 98, 7152-7158.	1.2	49
34	Polycyclic antiaromatic hydrocarbons. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 6630.	1.3	49
35	Electrostatic spectral tuning mechanism of the green fluorescent protein. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 4491.	1.3	47
36	Calculation of vibrationally resolved absorption spectra of acenes and pyrene. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 21094-21103.	1.3	47

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37	Two-dimensional, fully numerical molecular calculations. <i>Molecular Physics</i> , 1987, 60, 597-604.	0.8	45
38	Coupled-cluster and density functional theory studies of the electronic excitation spectra of trans-1,3-butadiene and trans-2-propeniminium. <i>Journal of Chemical Physics</i> , 2009, 131, 024301.	1.2	44
39	Gauge-Origin Independent Calculations of the Anisotropy of the Magnetically Induced Current Densities. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5658-5664.	1.1	44
40	The Effect of Protein Environment on Photoexcitation Properties of Retinal. <i>Journal of Physical Chemistry B</i> , 2012, 116, 2249-2258.	1.2	43
41	Spectral Tuning of Rhodopsin and Visual Cone Pigments. <i>Journal of the American Chemical Society</i> , 2014, 136, 2723-2726.	6.6	43
42	Calculations of current densities for neutral and doubly charged persubstituted benzenes using effective core potentials. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 7124-7131.	1.3	43
43	Benchmarking Magnetizabilities with Recent Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1457-1468.	2.3	43
44	Aromatic pathways in mono- and bisphosphorous singly Möbius twisted [28] and [30]hexaphyrins. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20659.	1.3	41
45	Computational Studies of Aromatic and Photophysical Properties of Expanded Porphyrins. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4756-4767.	1.1	41
46	A density-functional-theory study of bacteriochlorophyll b. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 4265.	1.3	40
47	Benchmarking the Approximate Second-Order Coupled-Cluster Method on Biochromophores. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2473-2484.	2.3	40
48	Closed-shell paramagnetic porphyrinoids. <i>Chemical Communications</i> , 2017, 53, 9866-9869.	2.2	40
49	The exactness of the extended Koopmans's theorem: A numerical study. <i>Journal of Chemical Physics</i> , 1993, 98, 3999-4002.	1.2	39
50	Current density and molecular magnetic properties. <i>Chemical Communications</i> , 2021, 57, 12362-12378.	2.2	39
51	A modified variation-perturbation approach to zero-point vibrational motion. <i>Theoretical Chemistry Accounts</i> , 2000, 103, 365-373.	0.5	38
52	Insights into Magnetically Induced Current Pathways and Optical Properties of Isophlorins. <i>Journal of Physical Chemistry A</i> , 2013, 117, 9062-9068.	1.1	38
53	Calculating rate constants for intersystem crossing and internal conversion in the Franck-Condon and Herzberg-Teller approximations. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 18495-18500.	1.3	38
54	Exploring the Stability of Golden Fullerenes. <i>Journal of Physical Chemistry C</i> , 2008, 112, 19311-19315.	1.5	37

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55	Relation Between Ring Currents and Hydrogenation Enthalpies for Assessing the Degree of Aromaticity. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7282-7289.	1.1	37
56	Magnetically Induced Currents in Bianthraquinodimethane-Stabilized Möbius and Hückel [16]Annulenes. <i>Journal of Organic Chemistry</i> , 2009, 74, 6495-6502.	1.7	36
57	Hydrogen-bond strengths by magnetically induced currents. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 434-437.	1.3	35
58	Importance of Vibronic Effects in the UV-Vis Spectrum of the 7,7,8,8-Tetracyanoquinodimethane Anion. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5058-5066.	2.3	35
59	Aromaticity of the doubly charged [8]circulenes. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 8980-8992.	1.3	34
60	Calculation of Magnetically Induced Currents in Hydrocarbon Nanorings. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13584-13592.	1.1	33
61	C72: gaudiene, a hollow and aromatic all-carbon molecule. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 9025.	1.3	33
62	Exploring the Light-Capturing Properties of Photosynthetic Chlorophyll Clusters Using Large-Scale Correlated Calculations. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2644-2651.	2.3	32
63	First-principles calculations of anharmonic and deuteration effects on the photophysical properties of polyacenes and porphyrinoids. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 22314-22323.	1.3	32
64	Tetraberyllium- I^{4+} -oxo-hexa(arylcarboxylates). <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2001, 56, 979-989.	0.3	31
65	Computational studies of ^{13}C NMR chemical shifts of saccharides. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 2561.	1.3	31
66	Coupled-Cluster Studies of Extensive Green Fluorescent Protein Models Using the Reduced Virtual Space Approach. <i>Journal of Physical Chemistry B</i> , 2015, 119, 2933-2945.	1.2	30
67	Aromaticity of Even-Number Cyclo[n]carbons ($n = 6-100$). <i>Journal of Physical Chemistry A</i> , 2020, 124, 10849-10855.	1.1	30
68	Aromatic pathways in thieno-bridged porphyrins: understanding the influence of the direction of the thiophene ring on the aromatic character. <i>Molecular Physics</i> , 2013, 111, 1364-1372.	0.8	29
69	Electronic and optical properties of metalloporphyrins of zinc on TiO_2 cluster in dye-sensitized solar-cells (DSSC). A quantum chemistry study. <i>RSC Advances</i> , 2017, 7, 42677-42684.	1.7	29
70	Two-dimensional, fully numerical molecular calculations. <i>Molecular Physics</i> , 1985, 55, 627-635.	0.8	28
71	New insights into aromatic pathways of carbachlorins and carbaporphyrins based on calculations of magnetically induced current densities. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 11932-11941.	1.3	28
72	Theoretical studies as a tool for understanding the aromatic character of porphyrinoid compounds. <i>Chemical Modelling</i> , 0, 1-42.	0.2	28

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73	Density functional studies of the luminescence of Si ₂₉ H ₃₆ . <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 2044.	1.3	27
74	Parallel implementation of a direct method for calculating electrostatic potentials. <i>Journal of Chemical Physics</i> , 2007, 126, 094101.	1.2	27
75	Predicting the degree of aromaticity of novel carbaporphyrinoids. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 14215-14222.	1.3	27
76	Novel hollow all-carbon structures. <i>Nanoscale</i> , 2015, 7, 15886-15894.	2.8	27
77	Universal method for computation of electrostatic potentials. <i>Journal of Chemical Physics</i> , 2005, 122, 194107.	1.2	26
78	On the Aromaticity of the Planar Hydrogen-Bonded (HF) ₃ Trimer. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 761-764.	2.3	26
79	The aromatic character of thienopyrrole-modified 20 π -electron porphyrinoids. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 11010.	1.3	26
80	[Hg ₄ Te ₈ (Te ₂) ₄] ⁸⁺ : A Heavy Metal Porphyrinoid Embedded in a Lamellar Structure. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 8770-8774.	7.2	26
81	The direct approach to gravitation and electrostatics method for periodic systems. <i>Journal of Chemical Physics</i> , 2010, 132, 024102.	1.2	24
82	A divide and conquer real-space approach for all-electron molecular electrostatic potentials and interaction energies. <i>Journal of Chemical Physics</i> , 2012, 136, 214104.	1.2	24
83	Aromatic Pathways in Carbathioporphyrins. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1201-1207.	1.1	23
84	Antiaromatic Character of 16 π Electron Octaethylporphyrins: Magnetically Induced Ring Currents from DFT-GIMIC Calculations. <i>Journal of Physical Chemistry A</i> , 2015, 119, 2344-2350.	1.1	23
85	Non-intersecting ring currents in [12]infinite. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 6404-6409.	1.3	23
86	Calculation of ring-current susceptibilities for potentially homoaromatic hydrocarbons. <i>Computational and Theoretical Chemistry</i> , 2003, 633, 123-136.	1.5	21
87	Bicycloaromaticity and Baird-type bicycloaromaticity of dithienothiophene-bridged [34]octaphyrins. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 17705-17713.	1.3	21
88	Ab Initio Studies of Triplet-State Properties for Organic Semiconductor Molecules. <i>Journal of Physical Chemistry C</i> , 2012, 116, 15203-15217.	1.5	20
89	Magnetically Induced Current Densities in Toroidal Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2019, 123, 15354-15365.	1.5	20
90	Aromatic pathways in conjugated rings connected by single bonds. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 848-857.	1.0	19

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91	Double Photoinduced Jahn–Teller Distortion of Tetrahedral Au ^I Sn ^{II} Complexes. <i>ChemPlusChem</i> , 2014, 79, 67-76.	1.3	19
92	Optical and magnetic properties of antiaromatic porphyrinoids. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 25979-25988.	1.3	19
93	Magnetically Induced Ring-Current Strengths in Möbius Twisted Annulenes. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 1627-1632.	2.1	19
94	Fully numerical electronic structure calculations on diatomic molecules in weak to strong magnetic fields. <i>Molecular Physics</i> , 2020, 118, .	0.8	19
95	Calculations of current densities and aromatic pathways in cyclic porphyrin and isoporphyrin arrays. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 12794-12803.	1.3	18
96	Aromatic and Antiaromatic Pathways in Triphyrin(2.1.1) Annulated with Benzo[<i>b</i>]heterocycles. <i>Chemistry - A European Journal</i> , 2019, 25, 15477-15482.	1.7	18
97	When are Antiaromatic Molecules Paramagnetic?. <i>Journal of Physical Chemistry C</i> , 2020, 124, 21027-21035.	1.5	18
98	Atoms and molecules in soft confinement potentials. <i>Molecular Physics</i> , 2020, 118, e1730989.	0.8	18
99	Tuning the Protein-Induced Absorption Shifts of Retinal in Engineered Rhodopsin Mimics. <i>Chemistry - A European Journal</i> , 2016, 22, 8254-8261.	1.7	17
100	Interplay of Aromaticity and Antiaromaticity in N-Doped Nanographenes. <i>Journal of Physical Chemistry A</i> , 2020, 124, 695-703.	1.1	17
101	Spatial Contributions to Nuclear Magnetic Shieldings. <i>Journal of Physical Chemistry A</i> , 2021, 125, 1778-1786.	1.1	17
102	Magnetically Induced Ring-Current Strengths of Planar and Nonplanar Molecules: New Insights from the Pseudo- π Model. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5753-5764.	1.1	17
103	Full configuration interaction studies of phonon and photon transition rates in semiconductor quantum dots. <i>Molecular Physics</i> , 2002, 100, 911-918.	0.8	16
104	Relations between the aromaticity and magnetic dipole transitions in the electronic spectra of hetero[8]circulenes. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 30239-30246.	1.3	16
105	Absorption shifts of diastereotopically ligated chlorophyll dimers of photosystem I. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 6851-6858.	1.3	16
106	Fast estimation of the internal conversion rate constant in photophysical applications. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 6344-6348.	1.3	16
107	Coupled-cluster calculations of the lowest $\sigma^* \leftarrow \sigma$ bands of the electronic excitation spectrum of naphthalene. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 9859.	1.3	15
108	Evaluating Shielding-Based Ring-Current Models by Using the Gauge-Including Magnetically Induced Current Method. <i>Journal of the Chinese Chemical Society</i> , 2016, 63, 93-100.	0.8	15

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109	The influence of heteroatoms on the aromatic character and the current pathways of B ₂ N ₂ -dibenzo[a,e]pentalenes. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 20213-20223.	1.3	15
110	Perhalophenyl Three-Coordinate Gold(I) Complexes as TADF Emitters: A Photophysical Study from Experimental and Computational Viewpoints. <i>Inorganic Chemistry</i> , 2020, 59, 14236-14244.	1.9	15
111	Integration of global ring currents using the Ampère-Maxwell law. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 624-628.	1.3	15
112	Coupled-cluster and density functional theory studies of the electronic $\pi \rightarrow \pi^*$ transitions of the DNA bases. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 6931-6941.	1.3	14
113	Magnetic response properties of gaudiene – a cavernous and aromatic carbocage. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 18880-18886.	1.3	14
114	The aromatic character of [10]annulenes and dicupra[10]annulenes from current density calculations. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 1337-1346.	1.3	14
115	Response to – Comment on – The exactness of the extended Koopmans’ theorem: A numerical study [J. Chem. Phys. 99, 6221 (1993)]. <i>Journal of Chemical Physics</i> , 1993, 99, 6222-6223.	1.2	13
116	The Quest for Beryllium Peroxides. <i>Inorganic Chemistry</i> , 2001, 40, 2270-2274.	1.9	13
117	Full Configuration Interaction Calculations of Electron-Hole Correlation Effects in Strain-Induced Quantum Dots. <i>Physica Status Solidi (B): Basic Research</i> , 2001, 224, 775-779.	0.7	13
118	The grid-based fast multipole method – a massively parallel numerical scheme for calculating two-electron interaction energies. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 31480-31490.	1.3	13
119	Insights into Molecular Structures and Optical Properties of Stacked [Au ₃ (RN=C ₂) ₃] _n Complexes. <i>Inorganic Chemistry</i> , 2018, 57, 718-730.	1.9	13
120	On the Mechanism of the Reactivity of 1,3-Dialkylimidazolium Salts under Basic to Acidic Conditions: A Combined Kinetic and Computational Study. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 11613-11617.	7.2	13
121	Calculation of vibrationally resolved absorption and fluorescence spectra of the rylenes. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 2379-2385.	1.3	13
122	Core-electron contributions to the molecular magnetic response. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 12158-12166.	1.3	13
123	Nuclear Magnetic Shieldings of Stacked Aromatic and Antiaromatic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1952-1962.	2.3	12
124	An Ab Initio Study of Structure and Energetics of Free-Base Bonellin-Dimethylester Isomers and Transition States. <i>Chemistry - A European Journal</i> , 1999, 5, 267-273.	1.7	11
125	Theoretical investigation of photoelectron spectra and magnetically induced current densities in ring-shaped transition-metal oxides. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 701-713.	0.5	11
126	Construction of the Fock Matrix on a Grid-Based Molecular Orbital Basis Using GPGPUs. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2053-2062.	2.3	11

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127	Carrier-Carrier Correlations in Strain-Induced Quantum Dots. <i>Physica Status Solidi (B): Basic Research</i> , 2000, 221, 37-41.	0.7	10
128	Aromaticity Indices from Magnetic Shieldings. , 2004, , 395-407.		10
129	Calculation of magnetic response properties of tetrazines. <i>RSC Advances</i> , 2020, 10, 18124-18130.	1.7	10
130	Computational methods for studies of multiexciton complexes. <i>Physica Status Solidi (B): Basic Research</i> , 2006, 243, 4035-4045.	0.7	9
131	Thiolate-protected golden fullerenes. A 32-ve core involving a hollow Au ₃₂ cage. <i>RSC Advances</i> , 2016, 6, 21332-21336.	1.7	9
132	A Generalized Grid-Based Fast Multipole Method for Integrating Helmholtz Kernels. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 654-665.	2.3	9
133	[Hg ₄ Te ₈ (Te ₂) ₄] ⁸⁻ : ein Schwermetall-Porphyrinoid in einer lamellaren Struktur. <i>Angewandte Chemie</i> , 2018, 130, 8906-8910.	1.6	9
134	Magnetically induced ring currents in metallocenothiaporphyrins. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1666-1674.	1.3	9
135	Calculations of the light absorption spectra of porphyrinoid chromophores for dye-sensitized solar cells. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27877-27884.	1.3	8
136	Aromaticity introduced by antiferromagnetic ligand mediated metal-metal interactions. Insights from the induced magnetic response in [Cu ₆ (dmPz) ₆ (OH) ₆]. <i>Inorganic Chemistry Frontiers</i> , 2017, 4, 986-993.	3.0	8
137	Computational methods for studies of semiconductor quantum dots and rings. <i>Annual Reports on the Progress of Chemistry Section C</i> , 2012, 108, 96.	4.4	7
138	Computational studies of the corrosion-inhibition efficiency of iron by triazole surfactants. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1365-1371.	1.0	7
139	Solvation chemical shifts of perylenic antenna molecules from molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 22309-22320.	1.3	7
140	Optimization of numerical orbitals using the Helmholtz kernel. <i>Journal of Chemical Physics</i> , 2017, 146, 084102.	1.2	7
141	Divergent Carbocatalytic Routes in Oxidative Coupling of Benzofused Heteroaryl Dimers: A Mechanistic Update. <i>Chemistry - A European Journal</i> , 2021, 27, 5283-5291.	1.7	7
142	Influence of perhalophenyl groups in the TADF mechanism of diphosphino gold complexes. <i>Journal of Materials Chemistry C</i> , 2022, 10, 4894-4904.	2.7	7
143	Magnetically Induced Current Densities in Zinc Porphyrin Nanoshells. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1936-1945.	1.1	7
144	Odd-Number Cyclo[n]Carbons Sustaining Alternating Aromaticity. <i>Journal of Physical Chemistry A</i> , 2022, 126, 2445-2452.	1.1	7

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145	Sphere Currents of Buckminsterfullerene. <i>Angewandte Chemie</i> , 2005, 117, 1877-1880.	1.6	6
146	Double Jahn-Teller Distortion in AuGe Complexes Leading to a Dual Blue-Orange Emission. <i>ChemPlusChem</i> , 2016, 81, 176-186.	1.3	6
147	The Excitation Spectra of Naphthalene Dimers: Frenkel and Charge-transfer Excitons. <i>Journal of the Chinese Chemical Society</i> , 2016, 63, 20-32.	0.8	6
148	Relation between molecular electronic structure and nuclear spin-induced circular dichroism. <i>Scientific Reports</i> , 2017, 7, 46617.	1.6	6
149	Density Functional Theory under the Bubbles and Cube Numerical Framework. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4237-4245.	2.3	6
150	Deacetylation of per-acetylated glycopyranosides: An overall pattern for acidic catalysis. <i>Chemical Physics Letters</i> , 2019, 723, 123-127.	1.2	6
151	Spatial Contributions to ¹ H NMR Chemical Shifts of Free-Base Porphyrinoids. <i>Chemistry</i> , 2021, 3, 1005-1021.	0.9	6
152	Construction of the two-electron contribution to the Fock matrix by numerical integration. <i>Molecular Physics</i> , 2012, 110, 2569-2578.	0.8	5
153	Computational and experimental studies of the electronic excitation spectra of EDTA and DTPA substituted tetraphenylporphyrins and their Lu complexes. <i>Journal of Molecular Modeling</i> , 2013, 19, 4631-4637.	0.8	5
154	The aromaticity of verdazyl radicals and their closed-shell charged species. <i>New Journal of Chemistry</i> , 2018, 42, 19987-19994.	1.4	5
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