Dage Matts BÃ¶rje Sundholm

List of Publications by Year
in descending order

176 papers	6,637 citations	70961 41 h-index	79541 73 g-index
181 all docs	181 docs citations	181 times ranked	4111 citing authors

#	Article	IF	Citations
1	Aromatic Pathways in Porphyrinoids by Magnetically Induced Ring Currents. Handbook of Porphyrin Science, 2022, , 1-39.	0.3	1
2	Influence of perhalophenyl groups in the TADF mechanism of diphosphino gold(<scp>i</scp>) complexes. Journal of Materials Chemistry C, 2022, 10, 4894-4904.	2.7	7
3	Integration of global ring currents using the AmpÃ¨reâ€“Maxwell law. Physical Chemistry Chemical Physics, 2022, 24, 624-628.	1.3	15
4	Magnetically induced ring currents in metallocenothiaporphyrins. Physical Chemistry Chemical Physics, 2022, 24, 1666-1674.	1.3	9
5	Non-intersecting ring currents in [12]infinitene. Physical Chemistry Chemical Physics, 2022, 24, 6404-6409.	1.3	23
6	Magnetically Induced Current Densities in Zinc Porphyrin Nanoshells. Journal of Physical Chemistry A, 2022, 126, 1936-1945.	1.1	7
7	Core-electron contributions to the molecular magnetic response. Physical Chemistry Chemical Physics, 2022, 24, 12158-12166.	1.3	13
8	Odd-Number Cyclo[n]Carbons Sustaining Alternating Aromaticity. Journal of Physical Chemistry A, 2022, 126, 2445-2452.	1.1	7
9	Diagnosing Ring Current(s) in Figure-Eight Skeletons: A 3D Through-Space Conjugation in the Two-Loops Crossing. Organic Letters, 2022, 24, 4876-4880.	2.4	4
10	Magnetically induced ring currents in naphthalene-fused heteroporphyrinoids. Physical Chemistry Chemical Physics, 2021, 23, 16629-16634.	1.3	2
11	Fast estimation of the internal conversion rate constant in photophysical applications. Physical Chemistry Chemical Physics, 2021, 23, 6344-6348.	1.3	16
12	Current density, current-density pathways, and molecular aromaticity. , 2021, , 155-194.		4
13	Spatial Contributions to Nuclear Magnetic Shieldings. Journal of Physical Chemistry A, 2021, 125, 1778-1786.	1.1	17
14	Benchmarking Magnetizabilities with Recent Density Functionals. Journal of Chemical Theory and Computation, 2021, 17, 1457-1468.	2.3	43
15	Divergent Carbocatalytic Routes in Oxidative Coupling of Benzofused Heteroaryl Dimers: A Mechanistic Update. Chemistry - A European Journal, 2021, 27, 5283-5291.	1.7	7
16	Magnetically Induced Ring-Current Strengths of Planar and Nonplanar Molecules: New Insights from the Pseudo-Î€ Model. Journal of Physical Chemistry A, 2021, 125, 5753-5764.	1.1	17
17	Spatial Contributions to 1H NMR Chemical Shifts of Free-Base Porphyrinoids. Chemistry, 2021, 3, 1005-1021.	0.9	6
18	Current density and molecular magnetic properties. Chemical Communications, 2021, 57, 12362-12378.	2.2	39

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19	Fully numerical electronic structure calculations on diatomic molecules in weak to strong magnetic fields. Molecular Physics, 2020, 118, .	0.8	19
20	Benchmarking the Performance of Time-Dependent Density Functional Theory Methods on Biochromophores. Journal of Chemical Theory and Computation, 2020, 16, 587-600.	2.3	69
21	Perhalophenyl Three-Coordinate Gold(I) Complexes as TADF Emitters: A Photophysical Study from Experimental and Computational Viewpoints. Inorganic Chemistry, 2020, 59, 14236-14244.	1.9	15
22	The effect of anion complexation on the aromatic properties of aromatic and antiaromatic porphyrinoids. New Journal of Chemistry, 2020, 44, 20643-20650.	1.4	4
23	When are Antiaromatic Molecules Paramagnetic?. Journal of Physical Chemistry C, 2020, 124, 21027-21035.	1.5	18
24	First-principles calculations of anharmonic and deuteration effects on the photophysical properties of polyacenes and porphyrinoids. Physical Chemistry Chemical Physics, 2020, 22, 22314-22323.	1.3	32
25	Aromaticity of Even-Number Cyclo[n]carbons (n = 6â€“100). Journal of Physical Chemistry A, 2020, 124, 10849-10855.	1.1	30
26	Calculation of magnetic response properties of tetrazines. RSC Advances, 2020, 10, 18124-18130.	1.7	10
27	Atoms and molecules in soft confinement potentials. Molecular Physics, 2020, 118, e1730989.	0.8	18
28	Interplay of Aromaticity and Antiaromaticity in N-Doped Nanographenes. Journal of Physical Chemistry A, 2020, 124, 695-703.	1.1	17
29	Calculation of vibrationally resolved absorption and fluorescence spectra of the rylenes. Physical Chemistry Chemical Physics, 2020, 22, 2379-2385.	1.3	13
30	A method for designing a novel class of gold-containing molecules. Chemical Communications, 2020, 56, 5433-5436.	2.2	5
31	Photophysical properties of the triangular [Au(HNî€COH)]₃ complex and its dimer. Physical Chemistry Chemical Physics, 2020, 22, 10314-10321.	1.3	3
32	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.	1.3	38
33	Ab Initio Study of Phosphorescence of Hetero[8]Circulenes. Russian Physics Journal, 2019, 62, 406-410.	0.2	2
34	Cyclo[18]carbon: Insight into Electronic Structure, Aromaticity, and Surface Coupling. Journal of Physical Chemistry Letters, 2019, 10, 6701-6705.	2.1	103
35	Aromatic and Antiaromatic Pathways in Triphyrin(2.1.1) Annelated with Benzo[b]heterocycles. Chemistry - A European Journal, 2019, 25, 15477-15482.	1.7	18
36	Predicting Stable Molecular Structures for (RNC)₂Au^IX Complexes. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2019, 645, 1127-1134.	0.6	0

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37	Calculation of vibrationally resolved absorption spectra of acenes and pyrene. Physical Chemistry Chemical Physics, 2019, 21, 21094-21103.	1.3	47
38	Magnetically Induced Current Densities in Toroidal Carbon Nanotubes. Journal of Physical Chemistry C, 2019, 123, 15354-15365.	1.5	20
39	Deacetylation of per-acetatylated glycopyranosides: An overall pattern for acidic catalyzis. Chemical Physics Letters, 2019, 723, 123-127.	1.2	6
40	Absorption shifts of diastereotopically ligated chlorophyll dimers of photosystem I. Physical Chemistry Chemical Physics, 2019, 21, 6851-6858.	1.3	16
41	Aromatic Pathways in Porphycene Derivatives Based on Current-Density Calculations. Journal of Physical Chemistry A, 2019, 123, 284-292.	1.1	1
42	First-principles method for calculating the rate constants of internal-conversion and intersystem-crossing transitions. Physical Chemistry Chemical Physics, 2018, 20, 6121-6133.	1.3	79
43	Insights into Molecular Structures and Optical Properties of Stacked [Au₃(RNâ•CRâ€²)₃]_n Complexes. Inorganic Chemistry, 2018, 57, 718-730.	1.9	13
44	Magnetically Induced Ring-Current Strengths in MÃ¶bius Twisted Annulenes. Journal of Physical Chemistry Letters, 2018, 9, 1627-1632.	2.1	19
45	The argon nuclear quadrupole moments. Molecular Physics, 2018, 116, 1682-1686.	0.8	2
46	The aromatic character of [10]annulenes and dicupra[10]annulenes from current density calculations. Physical Chemistry Chemical Physics, 2018, 20, 1337-1346.	1.3	14
47	Relations between the aromaticity and magnetic dipole transitions in the electronic spectra of hetero[8]circulenes. Physical Chemistry Chemical Physics, 2018, 20, 30239-30246.	1.3	16
48	The aromaticity of verdazyl radicals and their closed-shell charged species. New Journal of Chemistry, 2018, 42, 19987-19994.	1.4	5
49	Density Functional Theory under the Bubbles and Cube Numerical Framework. Journal of Chemical Theory and Computation, 2018, 14, 4237-4245.	2.3	6
50	Bicycloaromaticity and Baird-type bicycloaromaticity of dithienothiophene-bridged [34]octaphyrins. Physical Chemistry Chemical Physics, 2018, 20, 17705-17713.	1.3	21
51	On the Mechanism of the Reactivity of 1,3â€Dialkylimidazolium Salts under Basic to Acidic Conditions: A Combined Kinetic and Computational Study. Angewandte Chemie, 2018, 130, 11787-11791.	1.6	4
52	On the Mechanism of the Reactivity of 1,3â€Dialkylimidazolium Salts under Basic to Acidic Conditions: A Combined Kinetic and Computational Study. Angewandte Chemie - International Edition, 2018, 57, 11613-11617.	7.2	13
53	[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.	7.2	26
54	Computational Studies of Aromatic and Photophysical Properties of Expanded Porphyrins. Journal of Physical Chemistry A, 2018, 122, 4756-4767.	1.1	41

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55	Tensor decompositions for the bubbles and cube numerical framework. Computer Physics Communications, 2018, 232, 98-103.	3.0	3
56	[Hg 4 Te 8 (Te 2) 4] 8â˜ : ein Schwermetallâ€Porphyrinoid in einer lamellaren Struktur. Angewandte Chemie, 2018, 130, 8906-8910.	1.6	9
57	A Generalized Grid-Based Fast Multipole Method for Integrating Helmholtz Kernels. Journal of Chemical Theory and Computation, 2017, 13, 654-665.	2.3	9
58	Calculations of current densities for neutral and doubly charged persubstituted benzenes using effective core potentials. Physical Chemistry Chemical Physics, 2017, 19, 7124-7131.	1.3	43
59	Calculations of current densities and aromatic pathways in cyclic porphyrin and isoporphyrin arrays. Physical Chemistry Chemical Physics, 2017, 19, 12794-12803.	1.3	18
60	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.	3.3	73
61	Aromaticity introduced by antiferromagnetic ligand mediated metalâ€“metal interactions. Insights from the induced magnetic response in [Cu₆(dmPz)₆(OH)₆]. Inorganic Chemistry Frontiers, 2017, 4, 986-993.	3.0	8
62	Optimization of numerical orbitals using the Helmholtz kernel. Journal of Chemical Physics, 2017, 146, 084102.	1.2	7
63	Nuclear Magnetic Shieldings of Stacked Aromatic and Antiaromatic Molecules. Journal of Chemical Theory and Computation, 2017, 13, 1952-1962.	2.3	12
64	Closed-shell paramagnetic porphyrinoids. Chemical Communications, 2017, 53, 9866-9869.	2.2	40
65	Relation Between Ring Currents and Hydrogenation Enthalpies for Assessing the Degree of Aromaticity. Journal of Physical Chemistry A, 2017, 121, 7282-7289.	1.1	37
66	Optical and magnetic properties of antiaromatic porphyrinoids. Physical Chemistry Chemical Physics, 2017, 19, 25979-25988.	1.3	19
67	Relation between molecular electronic structure and nuclear spin-induced circular dichroism. Scientific Reports, 2017, 7, 46617.	1.6	6
68	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.	1.3	15
69	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.	1.7	29
70	Calculations of magnetically induced current densities: theory and applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 639-678.	6.2	244
71	Double Jahnâ€“Teller Distortion in AuGe Complexes Leading to a Dual Blueâ€“Orange Emission. ChemPlusChem, 2016, 81, 176-186.	1.3	6
72	Exploring the Light-Capturing Properties of Photosynthetic Chlorophyll Clusters Using Large-Scale Correlated Calculations. Journal of Chemical Theory and Computation, 2016, 12, 2644-2651.	2.3	32

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73	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.	2.3	35
74	Calculations of the light absorption spectra of porphyrinoid chromophores for dye-sensitized solar cells. Physical Chemistry Chemical Physics, 2016, 18, 27877-27884.	1.3	8
75	Double Jahn-Teller Distortion in AuGe Complexes Leading to a Dual Blue-Orange Emission. ChemPlusChem, 2016, 81, 156-156.	1.3	0
76	The Excitation Spectra of Naphthalene Dimers: Frenkel and Chargeâ€transfer Excitons. Journal of the Chinese Chemical Society, 2016, 63, 20-32.	0.8	6
77	Cover Image, Volume 6, Issue 6. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, i.	6.2	0
78	Gauge-Origin Independent Calculations of the Anisotropy of the Magnetically Induced Current Densities. Journal of Physical Chemistry A, 2016, 120, 5658-5664.	1.1	44
79	Magnetic response properties of gaudiene â€“ a cavernous and aromatic carbocage. Physical Chemistry Chemical Physics, 2016, 18, 18880-18886.	1.3	14
80	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.	1.3	61
81	Tuning the Proteinâ€Induced Absorption Shifts of Retinal in Engineered Rhodopsin Mimics. Chemistry - A European Journal, 2016, 22, 8254-8261.	1.7	17
82	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.	0.8	15
83	Thiolate-protected golden fullerenes. A 32-ve core involving a hollow Au₃₂cage. RSC Advances, 2016, 6, 21332-21336.	1.7	9
84	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.	1.3	28
85	Aromaticity of the doubly charged [8]circulenes. Physical Chemistry Chemical Physics, 2016, 18, 8980-8992.	1.3	34
86	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.	1.3	13
87	Computational Studies of a Paramagnetic Planar Dibenzotetraaza[14]annulene Ni(II) Complex. Journal of Physical Chemistry A, 2015, 119, 5189-5196.	1.1	4
88	Aromatic Pathways in Carbathiaporphyrins. Journal of Physical Chemistry A, 2015, 119, 1201-1207.	1.1	23
89	Coupled-Cluster Studies of Extensive Green Fluorescent Protein Models Using the Reduced Virtual Space Approach. Journal of Physical Chemistry B, 2015, 119, 2933-2945.	1.2	30
90	Construction of the Fock Matrix on a Grid-Based Molecular Orbital Basis Using GPGPUs. Journal of Chemical Theory and Computation, 2015, 11, 2053-2062.	2.3	11

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91	Predicting the degree of aromaticity of novel carbaporphyrinoids. Physical Chemistry Chemical Physics, 2015, 17, 14215-14222.	1.3	27
92	Proteinâ€Induced Color Shift of Carotenoids in Î²â€Crustacyanin. Angewandte Chemie - International Edition, 2015, 54, 11564-11566.	7.2	57
93	Novel hollow all-carbon structures. Nanoscale, 2015, 7, 15886-15894.	2.8	27
94	Antiaromatic Character of 16 Ï€ Electron Octaethylporphyrins: Magnetically Induced Ring Currents from DFT-GIMIC Calculations. Journal of Physical Chemistry A, 2015, 119, 2344-2350.	1.1	23
95	On energetic prerequisites of attracting electrons. Journal of Chemical Physics, 2014, 140, 234111.	1.2	0
96	Double Photoinduced Jahnâ€“Teller Distortion of Tetrahedral Au^Iï£¿Sn^{II} Complexes. ChemPlusChem, 2014, 79, 67-76.	1.3	19
97	Coupled-cluster and density functional theory studies of the electronic 0â€“0 transitions of the DNA bases. Physical Chemistry Chemical Physics, 2014, 16, 6931-6941.	1.3	14
98	Coupled-cluster calculations of the lowest 0â€“0 bands of the electronic excitation spectrum of naphthalene. Physical Chemistry Chemical Physics, 2014, 16, 9859.	1.3	15
99	Solvation chemical shifts of perylenic antenna molecules from molecular dynamics simulations. Physical Chemistry Chemical Physics, 2014, 16, 22309-22320.	1.3	7
100	A comment to â€˜Catalyst Induced Hydrino Transition (CIHT) electrochemical cellâ€™. International Journal of Energy Research, 2014, 38, 1766-1766.	2.2	0
101	The aromatic character of thienopyrrole-modified 20Ï€-electron porphyrinoids. Physical Chemistry Chemical Physics, 2014, 16, 11010.	1.3	26
102	Spectral Tuning of Rhodopsin and Visual Cone Pigments. Journal of the American Chemical Society, 2014, 136, 2723-2726.	6.6	43
103	Computational and experimental studies of the electronic excitation spectra of EDTA and DTPA substituted tetraphenylporphyrins and their Lu complexes. Journal of Molecular Modeling, 2013, 19, 4631-4637.	0.8	5
104	Insights into Magnetically Induced Current Pathways and Optical Properties of Isophlorins. Journal of Physical Chemistry A, 2013, 117, 9062-9068.	1.1	38
105	An efficient algorithm to calculate three-electron integrals for Gaussian-type orbitals using numerical integration. Molecular Physics, 2013, 111, 2536-2543.	0.8	4
106	C72: gaudiene, a hollow and aromatic all-carbon molecule. Physical Chemistry Chemical Physics, 2013, 15, 9025.	1.3	33
107	Electrostatic spectral tuning mechanism of the green fluorescent protein. Physical Chemistry Chemical Physics, 2013, 15, 4491.	1.3	47
108	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.	0.8	29

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109	Computational studies of the corrosionâ€inhibition efficiency of iron by triazole surfactants. International Journal of Quantum Chemistry, 2013, 113, 1365-1371.	1.0	7
110	A divide and conquer real-space approach for all-electron molecular electrostatic potentials and interaction energies. Journal of Chemical Physics, 2012, 136, 214104.	1.2	24
111	Aromatic Pathways of Porphins, Chlorins, and Bacteriochlorins. Journal of Organic Chemistry, 2012, 77, 3408-3414.	1.7	80
112	Effect of Fluorine Substitution on the Aromaticity of Polycyclic Hydrocarbons. Journal of Physical Chemistry A, 2012, 116, 10257-10268.	1.1	57
113	Construction of the two-electron contribution to the Fock matrix by numerical integration. Molecular Physics, 2012, 110, 2569-2578.	0.8	5
114	The Effect of Protein Environment on Photoexcitation Properties of Retinal. Journal of Physical Chemistry B, 2012, 116, 2249-2258.	1.2	43
115	Ab Initio Studies of Triplet-State Properties for Organic Semiconductor Molecules. Journal of Physical Chemistry C, 2012, 116, 15203-15217.	1.5	20
116	Computational methods for studies of semiconductor quantum dots and rings. Annual Reports on the Progress of Chemistry Section C, 2012, 108, 96.	4.4	7
117	Computational studies of photophysical properties of porphin, tetraphenylporphyrin and tetrabenzoporphyrin. Physical Chemistry Chemical Physics, 2012, 14, 11508.	1.3	56
118	Aromatic pathways in mono- and bisphosphorous singly MÃ¶bius twisted [28] and [30]hexaphyrins. Physical Chemistry Chemical Physics, 2011, 13, 20659.	1.3	41
119	Benchmarking the Approximate Second-Order Coupled-Cluster Method on Biochromophores. Journal of Chemical Theory and Computation, 2011, 7, 2473-2484.	2.3	40
120	Calculation of spin-current densities using gauge-including atomic orbitals. Journal of Chemical Physics, 2011, 134, 054123.	1.2	109
121	The gauge including magnetically induced current method. Physical Chemistry Chemical Physics, 2011, 13, 20500.	1.3	326
122	Hydrogen-bond strengths by magnetically induced currents. Physical Chemistry Chemical Physics, 2011, 13, 434-437.	1.3	35
123	Reduction of the virtual space for coupled-cluster excitation energies of large molecules and embedded systems. Journal of Chemical Physics, 2011, 134, 214114.	1.2	55
124	Theoretical investigation of photoelectron spectra and magnetically induced current densities in ring-shaped transition-metal oxides. Theoretical Chemistry Accounts, 2011, 129, 701-713.	0.5	11
125	Aromatic pathways in conjugated rings connected by single bonds. International Journal of Quantum Chemistry, 2011, 111, 848-857.	1.0	19
126	The direct approach to gravitation and electrostatics method for periodic systems. Journal of Chemical Physics, 2010, 132, 024102.	1.2	24

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127	Magnetically Induced Currents in [n]Cycloparaphenylenes, n = 6â^'11. Journal of Organic Chemistry, 2010, 75, 5867-5874.	1.7	56
128	Aromatic Pathways in Twisted Hexaphyrins. Journal of Physical Chemistry A, 2010, 114, 7153-7161.	1.1	65
129	Calculation of absorption and emission spectra of [n]cycloparaphenylenes: the reason for the large Stokes shift. Physical Chemistry Chemical Physics, 2010, 12, 2751.	1.3	53
130	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.	1.2	44
131	Magnetically Induced Current Densities in Aromatic, Antiaromatic, Homoaromatic, and Nonaromatic Hydrocarbons. Journal of Physical Chemistry A, 2009, 113, 8668-8676.	1.1	164
132	Magnetically Induced Currents in Bianthraquinodimethane-Stabilized MÃ¶bius and HÃ¼ckel [16]Annulenes. Journal of Organic Chemistry, 2009, 74, 6495-6502.	1.7	36
133	Calculation of Magnetically Induced Currents in Hydrocarbon Nanorings. Journal of Physical Chemistry A, 2008, 112, 13584-13592.	1.1	33
134	Polycyclic antiaromatic hydrocarbons. Physical Chemistry Chemical Physics, 2008, 10, 6630.	1.3	49
135	Exploring the Stability of Golden Fullerenes. Journal of Physical Chemistry C, 2008, 112, 19311-19315.	1.5	37
136	Parallel implementation of a direct method for calculating electrostatic potentials. Journal of Chemical Physics, 2007, 126, 094101.	1.2	27
137	On the Aromaticity of the Planar Hydrogen-Bonded (HF)3Trimer. Journal of Chemical Theory and Computation, 2006, 2, 761-764.	2.3	26
138	Computational methods for studies of multiexciton complexes. Physica Status Solidi (B): Basic Research, 2006, 243, 4035-4045.	0.7	9
139	Sphere Currents of Buckminsterfullerene. Angewandte Chemie - International Edition, 2005, 44, 1843-1846.	7.2	113
140	Sphere Currents of Buckminsterfullerene. Angewandte Chemie, 2005, 117, 1877-1880.	1.6	6
141	Universal method for computation of electrostatic potentials. Journal of Chemical Physics, 2005, 122, 194107.	1.2	26
142	Computational studies of 13C NMR chemical shifts of saccharides. Physical Chemistry Chemical Physics, 2005, 7, 2561.	1.3	31
143	Au32: A 24-Carat Golden Fullerene. Angewandte Chemie - International Edition, 2004, 43, 2678-2681.	7.2	285
144	Properties of WAu12. Physical Chemistry Chemical Physics, 2004, 6, 11-22.	1.3	97

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145	Density functional studies of the luminescence of Si29H36. Physical Chemistry Chemical Physics, 2004, 6, 2044.	1.3	27
146	Aromaticity Indices from Magnetic Shieldings. , 2004, , 395-407.		10
147	Calculation of current densities using gauge-including atomic orbitals. Journal of Chemical Physics, 2004, 121, 3952-3963.	1.2	393
148	Perturbation energy expansions based on two-component relativistic Hamiltonians. Theoretical Chemistry Accounts, 2003, 110, 144-152.	0.5	0
149	Calculation of ring-current susceptibilities for potentially homoaromatic hydrocarbons. Computational and Theoretical Chemistry, 2003, 633, 123-136.	1.5	21
150	A density-functional-theory study of bacteriochlorophyll b. Physical Chemistry Chemical Physics, 2003, 5, 4265.	1.3	40
151	Full configuration interaction studies of phonon and photon transition rates in semiconductor quantum dots. Molecular Physics, 2002, 100, 911-918.	0.8	16
152	The aromaticity and antiaromaticity of dehydroannulenes. Physical Chemistry Chemical Physics, 2001, 3, 2433-2437.	1.3	61
153	The Quest for Beryllium Peroxides. Inorganic Chemistry, 2001, 40, 2270-2274.	1.9	13
154	Full Configuration Interaction Calculations of Electron-Hole Correlation Effects in Strain-Induced Quantum Dots. Physica Status Solidi (B): Basic Research, 2001, 224, 775-779.	0.7	13
155	Tetraberyllium-Î·⁴-oxo-hexa(arylcarboxylates). Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2001, 56, 979-989.	0.3	31
156	Carrier-Carrier Correlations in Strain-Induced Quantum Dots. Physica Status Solidi (B): Basic Research, 2000, 221, 37-41.	0.7	10
157	A modified variation-perturbation approach to zero-point vibrational motion. Theoretical Chemistry Accounts, 2000, 103, 365-373.	0.5	38
158	Interpretation of the electronic absorption spectrum of free-base porphin using time-dependent density-functional theory. Physical Chemistry Chemical Physics, 2000, 2, 2275-2281.	1.3	109
159	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.	6.6	140
160	The Aromatic Character of Magnesium Porphyrins. Journal of Organic Chemistry, 2000, 65, 5233-5237.	1.7	83
161	The aromatic pathways of porphins, chlorins and bacteriochlorins. Physical Chemistry Chemical Physics, 2000, 2, 2145-2151.	1.3	99
162	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.	1.7	11

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163	Ab initio determination of the induced ring current in aromatic molecules. Physical Chemistry Chemical Physics, 1999, 1, 3429-3435.	1.3	173
164	Relativistic multiconfiguration Hartree-SFock by means of direct perturbation theory. International Journal of Quantum Chemistry, 1997, 65, 151-158.	1.0	2
165	A numerical Hartree-Fock program for diatomic molecules. Computer Physics Communications, 1996, 98, 346-358.	3.0	123
166	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.	1.2	49
167	The exactness of the extended Koopmansâ€™ theorem: A numerical study. Journal of Chemical Physics, 1993, 98, 3999-4002.	1.2	39
168	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.	1.2	13
169	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.	1.2	65
170	Two Fully Numerical Methods in Quantum Chemistry. International Journal of Modern Physics C, 1991, 02, 455-457.	0.8	2
171	Large multiconfigurational Hartree-Fock calculations on the hyperfine structure of Li(2S) and Li(2P). Physical Review A, 1990, 42, 2614-2621.	1.0	64
172	Two-dimensional, fully numerical molecular calculations. Molecular Physics, 1987, 60, 597-604.	0.8	45
173	Fully numerical hartree-fock methods for molecules. Computer Physics Reports, 1986, 4, 313-344.	2.3	240
174	Two-dimensional, fully numerical molecular calculations. Molecular Physics, 1985, 55, 627-635.	0.8	28
175	Two-dimensional, fully numerical molecular calculations. Molecular Physics, 1985, 56, 1411-1418.	0.8	113
176	Theoretical studies as a tool for understanding the aromatic character of porphyrinoid compounds. Chemical Modelling, 0, , 1-42.	0.2	28