Heike Fliegl

List of Publications by Year
in descending order

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66	4,006	196777	134545
papers	citations	29 h-index	62 g-index

67	67	67	3979
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Spatial Contributions to Nuclear Magnetic Shieldings. Journal of Physical Chemistry A, 2021, 125, 1778-1786.	1.1	17
2	Benchmarking Magnetizabilities with Recent Density Functionals. Journal of Chemical Theory and Computation, 2021, 17, 1457-1468.	2.3	43
3	Determinant Factors of Three-Dimensional Aromaticity in Antiaromatic Cyclophanes. Journal of the American Chemical Society, 2021, 143, 10676-10685.	6.6	38
4	Spatial Contributions to 1H NMR Chemical Shifts of Free-Base Porphyrinoids. Chemistry, 2021, 3, 1005-1021.	0.9	6
5	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
6	Tacticity dependence of single chain polymer folding. Polymer Chemistry, 2020, 11, 3439-3445.	1.9	5
7	Linking Optical and Magnetic Properties of (anti)Aromatic Porphyrinoids. ECS Meeting Abstracts, 2020, MA2020-01, 922-922.	0.0	0
8	Three-dimensional aromaticity in an antiaromatic cyclophane. Nature Communications, 2019, 10, 3576.	5.8	73
9	Calculation of vibrationally resolved absorption spectra of acenes and pyrene. Physical Chemistry Chemical Physics, 2019, 21, 21094-21103.	1.3	47
10	Four-component relativistic ³¹P NMR calculations for trans-platinum(<scp>ii</scp>) complexes: importance of the solvent and dynamics in spectral simulations. Dalton Transactions, 2019, 48, 8076-8083.	1.6	18
11	Ni(II) 10-Phosphacorrole: A Porphyrin Analogue Containing Phosphorus at the Meso Position. Journal of the American Chemical Society, 2019, 141, 4800-4805.	6.6	24
12	Absorption shifts of diastereotopically ligated chlorophyll dimers of photosystem I. Physical Chemistry Chemical Physics, 2019, 21, 6851-6858.	1.3	16
13	Magnetically Induced Ring-Current Strengths in MÃ¶bius Twisted Annulenes. Journal of Physical Chemistry Letters, 2018, 9, 1627-1632.	2.1	19
14	Bicycloaromaticity and Baird-type bicycloaromaticity of dithienothiophene-bridged [34]octaphyrins. Physical Chemistry Chemical Physics, 2018, 20, 17705-17713.	1.3	21
15	Rational Synthesis of Antiaromatic 5,15â€Dioxaporphyrin and Oxidation into Î²,Î²â€Linked Dimers. Angewandte Chemie, 2018, 130, 9876-9881.	1.6	12
16	Accelerating Kohnâ€Sham response theory using density fitting and the auxiliaryâ€densityâ€matrix method. International Journal of Quantum Chemistry, 2018, 118, e25639.	1.0	15
17	Computational Studies of Aromatic and Photophysical Properties of Expanded Porphyrins. Journal of Physical Chemistry A, 2018, 122, 4756-4767.	1.1	41
18	Rational Synthesis of Antiaromatic 5,15â€Dioxaporphyrin and Oxidation into Î²,Î²â€Linked Dimers. Angewandte Chemie - International Edition, 2018, 57, 9728-9733.	7.2	37

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19	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
20	Closed-shell paramagnetic porphyrinoids. Chemical Communications, 2017, 53, 9866-9869.	2.2	40
21	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
22	Optical and magnetic properties of antiaromatic porphyrinoids. Physical Chemistry Chemical Physics, 2017, 19, 25979-25988.	1.3	19
23	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
24	New Insights on Aromatic Pathways in Porphyrinoids. ECS Meeting Abstracts, 2017, , .	0.0	0
25	Calculations of magnetically induced current densities: theory and applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 639-678.	6.2	244
26	Nuclei-selected atomic-orbital response-theory formulation for the calculation of NMR shielding tensors using density-fitting. Journal of Chemical Physics, 2016, 145, 234108.	1.2	7
27	The Excitation Spectra of Naphthalene Dimers: Frenkel and Chargeâ€transfer Excitons. Journal of the Chinese Chemical Society, 2016, 63, 20-32.	0.8	6
28	Cover Image, Volume 6, Issue 6. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, i.	6.2	0
29	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
30	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
31	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
32	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
33	FemExâ€”female excellence in theoretical and computational chemistry. International Journal of Quantum Chemistry, 2015, 115, 1195-1196.	1.0	3
34	The origin dependence of the material constants: the permittivity and the inverse permeability. Molecular Physics, 2015, 113, 1899-1913.	0.8	7
35	Aromatic Pathways in Carbathiaporphyrins. Journal of Physical Chemistry A, 2015, 119, 1201-1207.	1.1	23
36	Predicting the degree of aromaticity of novel carbaporphyrinoids. Physical Chemistry Chemical Physics, 2015, 17, 14215-14222.	1.3	27

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37	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
38	Stereoselectivity through a network of non-classical CH weak interactions: a prospective study of a bicyclic organocatalytic scaffold. New Journal of Chemistry, 2014, 38, 5975-5982.	1.4	5
39	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	6.2	1,166
40	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
41	Unusual formation of a N-heterocyclic germylene via homolytic cleavage of a Câ€“C bond. Chemical Communications, 2014, 50, 3356-3358.	2.2	26
42	The aromatic character of thienopyrrole-modified 20Ï€-electron porphyrinoids. Physical Chemistry Chemical Physics, 2014, 16, 11010.	1.3	26
43	Mechanistic Insights on the Stereoselective Nucleophilic 1,2-Addition to Sulfinyl Imines. Journal of Organic Chemistry, 2014, 79, 2514-2521.	1.7	18
44	Insights into Magnetically Induced Current Pathways and Optical Properties of Isophlorins. Journal of Physical Chemistry A, 2013, 117, 9062-9068.	1.1	38
45	Heteroaromaticity approached by charge density investigations and electronic structure calculations. Physical Chemistry Chemical Physics, 2013, 15, 20600.	1.3	27
46	All-Metal Aromaticity: Revisiting the Ring Current Model among Transition Metal Clusters. Journal of Chemical Theory and Computation, 2013, 9, 4789-4796.	2.3	90
47	Non-perturbative treatment of molecules in linear magnetic fields: Calculation of anapole susceptibilities. Journal of Chemical Physics, 2013, 139, 164118.	1.2	31
48	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
49	Aromatic Pathways of Porphins, Chlorins, and Bacteriochlorins. Journal of Organic Chemistry, 2012, 77, 3408-3414.	1.7	80
50	Effect of Fluorine Substitution on the Aromaticity of Polycyclic Hydrocarbons. Journal of Physical Chemistry A, 2012, 116, 10257-10268.	1.1	57
51	Aromatic pathways in mono- and bisphosphorous singly MÃ¶bius twisted [28] and [30]hexaphyrins. Physical Chemistry Chemical Physics, 2011, 13, 20659.	1.3	41
52	The gauge including magnetically induced current method. Physical Chemistry Chemical Physics, 2011, 13, 20500.	1.3	326
53	Hydrogen-bond strengths by magnetically induced currents. Physical Chemistry Chemical Physics, 2011, 13, 434-437.	1.3	35
54	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

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55	Aromatic Pathways in Twisted Hexaphyrins. Journal of Physical Chemistry A, 2010, 114, 7153-7161.	1.1	65
56	Ridge-Tile-like Chiral Topology: Synthesis, Resolution, and Complete Chiroptical Characterization of Enantiomers of Edge-Sharing Binuclear Square Planar Complexes of Ni(II) Bearing Achiral Ligands. Journal of the American Chemical Society, 2010, 132, 10477-10483.	6.6	41
57	Magnetically Induced Current Densities in Aromatic, Antiaromatic, Homoaromatic, and Nonaromatic Hydrocarbons. Journal of Physical Chemistry A, 2009, 113, 8668-8676.	1.1	164
58	Expanding the Coordination Cage: A Ruthenium(II)â^'Polypyridine Complex Exhibiting High Quantum Yields under Ambient Conditions. Inorganic Chemistry, 2009, 48, 5677-5684.	1.9	73
59	Ab initio study of the magnetic exchange coupling constants of a structural model [CaMn3IIIMnII] of the oxygen evolving center in photosystem II. Physical Chemistry Chemical Physics, 2009, 11, 3900.	1.3	23
60	Calculation of Magnetically Induced Currents in Hydrocarbon Nanorings. Journal of Physical Chemistry A, 2008, 112, 13584-13592.	1.1	33
61	Inclusion of the (T) triples correction into the linear-r12 corrected coupled-cluster model CCSD(R12). International Journal of Quantum Chemistry, 2006, 106, 2306-2317.	1.0	69
62	Accurate computational determination of the binding energy of the SO3â^™H2O complex. Journal of Chemical Physics, 2006, 125, 054312.	1.2	30
63	Coupled-cluster response theory with linear-r12 corrections: The CC2-R12 model for excitation energies. Journal of Chemical Physics, 2006, 124, 044112.	1.2	48
64	Coupled-cluster theory with simplified linear-r12 corrections: The CCSD(R12) model. Journal of Chemical Physics, 2005, 122, 084107.	1.2	167
65	Ab Initio Calculation of the Vibrational and Electronic Spectra of trans- and cis-Azobenzene. Journal of the American Chemical Society, 2003, 125, 9821-9827.	6.6	194
66	Theoretical studies as a tool for understanding the aromatic character of porphyrinoid compounds. Chemical Modelling, 0, , 1-42.	0.2	28