Heike Fliegl

List of Publications by Year
in descending order

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66 papers	4,006 citations	172457 29 h-index	118850 62 g-index
67 all docs	67 docs citations	67 times ranked	3572 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	The gauge including magnetically induced current method. Physical Chemistry Chemical Physics, 2011, 13, 20500.	2.8	326
3	Calculations of magnetically induced current densities: theory and applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 639-678.	14.6	244
4	Ab Initio Calculation of the Vibrational and Electronic Spectra of trans- and cis-Azobenzene. Journal of the American Chemical Society, 2003, 125, 9821-9827.	13.7	194
5	Coupled-cluster theory with simplified linear-r12 corrections: The CCSD(R12) model. Journal of Chemical Physics, 2005, 122, 084107.	3.0	167
6	Magnetically Induced Current Densities in Aromatic, Antiaromatic, Homoaromatic, and Nonaromatic Hydrocarbons. Journal of Physical Chemistry A, 2009, 113, 8668-8676.	2.5	164
7	All-Metal Aromaticity: Revisiting the Ring Current Model among Transition Metal Clusters. Journal of Chemical Theory and Computation, 2013, 9, 4789-4796.	5.3	90
8	Aromatic Pathways of Porphins, Chlorins, and Bacteriochlorins. Journal of Organic Chemistry, 2012, 77, 3408-3414.	3.2	80
9	Expanding the Coordination Cage: A Ruthenium(II)â^'Polypyridine Complex Exhibiting High Quantum Yields under Ambient Conditions. Inorganic Chemistry, 2009, 48, 5677-5684.	4.0	73
10	Three-dimensional aromaticity in an antiaromatic cyclophane. Nature Communications, 2019, 10, 3576.	12.8	73
11	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.	2.0	69
12	Aromatic Pathways in Twisted Hexaphyrins. Journal of Physical Chemistry A, 2010, 114, 7153-7161.	2.5	65
13	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
14	Effect of Fluorine Substitution on the Aromaticity of Polycyclic Hydrocarbons. Journal of Physical Chemistry A, 2012, 116, 10257-10268.	2.5	57
15	Coupled-cluster response theory with linear-r12 corrections: The CC2-R12 model for excitation energies. Journal of Chemical Physics, 2006, 124, 044112.	3.0	48
16	Calculation of vibrationally resolved absorption spectra of acenes and pyrene. Physical Chemistry Chemical Physics, 2019, 21, 21094-21103.	2.8	47
17	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
18	Benchmarking Magnetizabilities with Recent Density Functionals. Journal of Chemical Theory and Computation, 2021, 17, 1457-1468.	5.3	43

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19	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.	13.7	41
20	Aromatic pathways in mono- and bisphosphorous singly MÃ¶bius twisted [28] and [30]hexaphyrins. Physical Chemistry Chemical Physics, 2011, 13, 20659.	2.8	41
21	Computational Studies of Aromatic and Photophysical Properties of Expanded Porphyrins. Journal of Physical Chemistry A, 2018, 122, 4756-4767.	2.5	41
22	Closed-shell paramagnetic porphyrinoids. Chemical Communications, 2017, 53, 9866-9869.	4.1	40
23	Insights into Magnetically Induced Current Pathways and Optical Properties of Isophlorins. Journal of Physical Chemistry A, 2013, 117, 9062-9068.	2.5	38
24	Determinant Factors of Three-Dimensional Aromaticity in Antiaromatic Cyclophanes. Journal of the American Chemical Society, 2021, 143, 10676-10685.	13.7	38
25	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
26	Rational Synthesis of Antiaromatic 5,15â€Dioxaporphyrin and Oxidation into Î²,Î²â€Linked Dimers. Angewandte Chemie - International Edition, 2018, 57, 9728-9733.	13.8	37
27	Hydrogen-bond strengths by magnetically induced currents. Physical Chemistry Chemical Physics, 2011, 13, 434-437.	2.8	35
28	Calculation of Magnetically Induced Currents in Hydrocarbon Nanorings. Journal of Physical Chemistry A, 2008, 112, 13584-13592.	2.5	33
29	Non-perturbative treatment of molecules in linear magnetic fields: Calculation of anapole susceptibilities. Journal of Chemical Physics, 2013, 139, 164118.	3.0	31
30	Accurate computational determination of the binding energy of the SO3â‹™H2O complex. Journal of Chemical Physics, 2006, 125, 054312.	3.0	30
31	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
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.	2.8	28
33	Theoretical studies as a tool for understanding the aromatic character of porphyrinoid compounds. Chemical Modelling, 0, , 1-42.	0.4	28
34	Heteroaromaticity approached by charge density investigations and electronic structure calculations. Physical Chemistry Chemical Physics, 2013, 15, 20600.	2.8	27
35	Predicting the degree of aromaticity of novel carbaporphyrinoids. Physical Chemistry Chemical Physics, 2015, 17, 14215-14222.	2.8	27
36	Unusual formation of a N-heterocyclic germylene via homolytic cleavage of a Câ€“C bond. Chemical Communications, 2014, 50, 3356-3358.	4.1	26

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37	The aromatic character of thienopyrrole-modified 20Ï€-electron porphyrinoids. Physical Chemistry Chemical Physics, 2014, 16, 11010.	2.8	26
38	Ni(II) 10-Phosphacorrole: A Porphyrin Analogue Containing Phosphorus at the Meso Position. Journal of the American Chemical Society, 2019, 141, 4800-4805.	13.7	24
39	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.	2.8	23
40	Aromatic Pathways in Carbathiaporphyrins. Journal of Physical Chemistry A, 2015, 119, 1201-1207.	2.5	23
41	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
42	Bicycloaromaticity and Baird-type bicycloaromaticity of dithienothiophene-bridged [34]octaphyrins. Physical Chemistry Chemical Physics, 2018, 20, 17705-17713.	2.8	21
43	Optical and magnetic properties of antiaromatic porphyrinoids. Physical Chemistry Chemical Physics, 2017, 19, 25979-25988.	2.8	19
44	Magnetically Induced Ring-Current Strengths in MÃ¶bius Twisted Annulenes. Journal of Physical Chemistry Letters, 2018, 9, 1627-1632.	4.6	19
45	Mechanistic Insights on the Stereoselective Nucleophilic 1,2-Addition to Sulfinyl Imines. Journal of Organic Chemistry, 2014, 79, 2514-2521.	3.2	18
46	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.	3.3	18
47	Spatial Contributions to Nuclear Magnetic Shieldings. Journal of Physical Chemistry A, 2021, 125, 1778-1786.	2.5	17
48	Absorption shifts of diastereotopically ligated chlorophyll dimers of photosystem I. Physical Chemistry Chemical Physics, 2019, 21, 6851-6858.	2.8	16
49	Coupled-cluster calculations of the lowest 0â€“0 bands of the electronic excitation spectrum of naphthalene. Physical Chemistry Chemical Physics, 2014, 16, 9859.	2.8	15
50	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
51	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
52	Accelerating Kohnâ€Sham response theory using density fitting and the auxiliaryâ€densityâ€matrix method. International Journal of Quantum Chemistry, 2018, 118, e25639.	2.0	15
53	Rational Synthesis of Antiaromatic 5,15â€Dioxaporphyrin and Oxidation into Î²,Î²â€Linked Dimers. Angewandte Chemie, 2018, 130, 9876-9881.	2.0	12
54	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

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55	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.	6.0	8
56	The origin dependence of the material constants: the permittivity and the inverse permeability. Molecular Physics, 2015, 113, 1899-1913.	1.7	7
57	Nuclei-selected atomic-orbital response-theory formulation for the calculation of NMR shielding tensors using density-fitting. Journal of Chemical Physics, 2016, 145, 234108.	3.0	7
58	The Excitation Spectra of Naphthalene Dimers: Frenkel and Chargeâ€transfer Excitons. Journal of the Chinese Chemical Society, 2016, 63, 20-32.	1.4	6
59	Spatial Contributions to 1H NMR Chemical Shifts of Free-Base Porphyrinoids. Chemistry, 2021, 3, 1005-1021.	2.2	6
60	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.	2.8	5
61	Tacticity dependence of single chain polymer folding. Polymer Chemistry, 2020, 11, 3439-3445.	3.9	5
62	The effect of anion complexation on the aromatic properties of aromatic and antiaromatic porphyrinoids. New Journal of Chemistry, 2020, 44, 20643-20650.	2.8	4
63	FemExâ€”female excellence in theoretical and computational chemistry. International Journal of Quantum Chemistry, 2015, 115, 1195-1196.	2.0	3
64	Cover Image, Volume 6, Issue 6. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, i.	14.6	0
65	New Insights on Aromatic Pathways in Porphyrinoids. ECS Meeting Abstracts, 2017, , .	0.0	0
66	Linking Optical and Magnetic Properties of (anti)Aromatic Porphyrinoids. ECS Meeting Abstracts, 2020, MA2020-01, 922-922.	0.0	0