

Heike Fliegl

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

62

papers

3,228

citations

26

h-index

56

g-index

67

ext. papers

3,634

ext. citations

4.8

avg, IF

5.31

L-index

#	Paper	IF	Citations
62	The Dalton quantum chemistry program system. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2014 , 4, 269-284	7.9	956
61	The gauge including magnetically induced current method. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 20500-18	3.6	231
60	Calculations of magnetically induced current densities: theory and applications. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2016 , 6, 639-678	7.9	174
59	Ab initio calculation of the vibrational and electronic spectra of trans- and cis-azobenzene. <i>Journal of the American Chemical Society</i> , 2003 , 125, 9821-7	16.4	168
58	Coupled-cluster theory with simplified linear-r(12) corrections: the CCSD(R12) model. <i>Journal of Chemical Physics</i> , 2005 , 122, 84107	3.9	158
57	Magnetically induced current densities in aromatic, antiaromatic, homoaromatic, and nonaromatic hydrocarbons. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 8668-76	2.8	138
56	All-Metal Aromaticity: Revisiting the Ring Current Model among Transition Metal Clusters. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 4789-96	6.4	75
55	Aromatic pathways of porphins, chlorins, and bacteriochlorins. <i>Journal of Organic Chemistry</i> , 2012 , 77, 3408-14	4.2	69
54	Expanding the coordination cage: a ruthenium(II)-polypyridine complex exhibiting high quantum yields under ambient conditions. <i>Inorganic Chemistry</i> , 2009 , 48, 5677-84	5.1	67
53	Inclusion of the (T) triples correction into the linear-r12 corrected coupled-cluster model CCSD(R12). <i>International Journal of Quantum Chemistry</i> , 2006 , 106, 2306-2317	2.1	66
52	Aromatic pathways in twisted hexaphyrins. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 7153-61	2.8	57
51	Effect of fluorine substitution on the aromaticity of polycyclic hydrocarbons. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 10257-68	2.8	50
50	Coupled-cluster response theory with linear-r12 corrections: the CC2-R12 model for excitation energies. <i>Journal of Chemical Physics</i> , 2006 , 124, 044112	3.9	46
49	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, 15934-42	3.6	43
48	Three-dimensional aromaticity in an antiaromatic cyclophane. <i>Nature Communications</i> , 2019 , 10, 3576	17.4	39
47	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. <i>Journal of the American Chemical Society</i> , 2010 , 132, 10477-83	16.4	39
46	Insights into magnetically induced current pathways and optical properties of isophlorins. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 9062-8	2.8	37

45	Aromatic pathways in mono- and bisphosphorous singly MBius twisted [28] and [30]hexaphyrins. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 20659-65	3.6	37
44	Gauge-Origin Independent Calculations of the Anisotropy of the Magnetically Induced Current Densities. <i>Journal of Physical Chemistry A</i> , 2016 , 120, 5658-64	2.8	35
43	Hydrogen-bond strengths by magnetically induced currents. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 434-7	3.6	34
42	Computational Studies of Aromatic and Photophysical Properties of Expanded Porphyrins. <i>Journal of Physical Chemistry A</i> , 2018 , 122, 4756-4767	2.8	33
41	Relation Between Ring Currents and Hydrogenation Enthalpies for Assessing the Degree of Aromaticity. <i>Journal of Physical Chemistry A</i> , 2017 , 121, 7282-7289	2.8	32
40	Calculation of magnetically induced currents in hydrocarbon nanorings. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 13584-92	2.8	32
39	Closed-shell paramagnetic porphyrinoids. <i>Chemical Communications</i> , 2017 , 53, 9866-9869	5.8	31
38	Heteroaromaticity approached by charge density investigations and electronic structure calculations. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 20600-10	3.6	27
37	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	1.7	27
36	Calculation of vibrationally resolved absorption spectra of acenes and pyrene. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 21094-21103	3.6	26
35	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, 11932-41	3.6	26
34	Accurate computational determination of the binding energy of the SO ₃ x H ₂ O complex. <i>Journal of Chemical Physics</i> , 2006 , 125, 054312	3.9	26
33	The aromatic character of thienopyrrole-modified 20 π -electron porphyrinoids. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 11010-6	3.6	25
32	Non-perturbative treatment of molecules in linear magnetic fields: calculation of anapole susceptibilities. <i>Journal of Chemical Physics</i> , 2013 , 139, 164118	3.9	25
31	Theoretical studies as a tool for understanding the aromatic character of porphyrinoid compounds. <i>Chemical Modelling</i> , 1-42	2	25
30	Predicting the degree of aromaticity of novel carbaporphyrinoids. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 14215-22	3.6	24
29	Antiaromatic character of 16 π -electron octaethylporphyrins: magnetically induced ring currents from DFT-GIMIC calculations. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 2344-50	2.8	23
28	Rational Synthesis of Antiaromatic 5,15-Dioxaporphyrin and Oxidation into π -Linked Dimers. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 9728-9733	16.4	23

27	Aromatic pathways in carbathiaporphyrins. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 1201-7	2.8	23
26	Unusual formation of a N-heterocyclic germylene via homolytic cleavage of a C-C bond. <i>Chemical Communications</i> , 2014 , 50, 3356-8	5.8	21
25	Ab initio study of the magnetic exchange coupling constants of a structural model [CaMn(3)(III)Mn(II)] of the oxygen evolving center in photosystem II. <i>Physical Chemistry Chemical Physics</i> , 2009 , 11, 3900-9	3.6	20
24	Benchmarking Magnetizabilities with Recent Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 1457-1468	6.4	19
23	Ni(II) 10-Phosphacorrole: A Porphyrin Analogue Containing Phosphorus at the Meso Position. <i>Journal of the American Chemical Society</i> , 2019 , 141, 4800-4805	16.4	17
22	Optical and magnetic properties of antiaromatic porphyrinoids. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 25979-25988	3.6	17
21	Bicycloaromaticity and Baird-type bicycloaromaticity of dithienothiophene-bridged [34]octaphyrins. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 17705-17713	3.6	17
20	Mechanistic insights on the stereoselective nucleophilic 1,2-addition to sulfinyl imines. <i>Journal of Organic Chemistry</i> , 2014 , 79, 2514-21	4.2	16
19	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	1.5	14
18	Coupled-cluster calculations of the lowest 0-0 bands of the electronic excitation spectrum of naphthalene. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 9859-65	3.6	14
17	Four-component relativistic P NMR calculations for trans-platinum(ii) complexes: importance of the solvent and dynamics in spectral simulations. <i>Dalton Transactions</i> , 2019 , 48, 8076-8083	4.3	13
16	Absorption shifts of diastereotopically ligated chlorophyll dimers of photosystem I. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 6851-6858	3.6	12
15	The influence of heteroatoms on the aromatic character and the current pathways of BN-dibenzo[a,e]pentalenes. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 20213-20223	3.6	12
14	Magnetically Induced Ring-Current Strengths in Möbius Twisted Annulenes. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 1627-1632	6.4	11
13	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	1.9	11
12	Determinant Factors of Three-Dimensional Aromaticity in Antiaromatic Cyclophanes. <i>Journal of the American Chemical Society</i> , 2021 , 143, 10676-10685	16.4	9
11	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	6.8	8
10	Accelerating Kohn-Sham response theory using density fitting and the auxiliary-density-matrix method. <i>International Journal of Quantum Chemistry</i> , 2018 , 118, e25639	2.1	8

9	Spatial Contributions to Nuclear Magnetic Shieldings. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 1778-1786	3.6	8
8	Rational Synthesis of Antiaromatic 5,15-Dioxaporphyrin and Oxidation into π -Linked Dimers. <i>Angewandte Chemie</i> , 2018 , 130, 9876-9881	3.6	7
7	The origin dependence of the material constants: the permittivity and the inverse permeability. <i>Molecular Physics</i> , 2015 , 113, 1899-1913	1.7	6
6	Nuclei-selected atomic-orbital response-theory formulation for the calculation of NMR shielding tensors using density-fitting. <i>Journal of Chemical Physics</i> , 2016 , 145, 234108	3.9	6
5	Stereoselectivity through a network of non-classical CH weak interactions: a prospective study of a bicyclic organocatalytic scaffold. <i>New Journal of Chemistry</i> , 2014 , 38, 5975-5982	3.6	4
4	The Excitation Spectra of Naphthalene Dimers: Frenkel and Charge-transfer Excitons. <i>Journal of the Chinese Chemical Society</i> , 2016 , 63, 20-32	1.5	3
3	Tacticity dependence of single chain polymer folding. <i>Polymer Chemistry</i> , 2020 , 11, 3439-3445	4.9	3
2	The effect of anion complexation on the aromatic properties of aromatic and antiaromatic porphyrinoids. <i>New Journal of Chemistry</i> , 2020 , 44, 20643-20650	3.6	2
1	Spatial Contributions to ¹ H NMR Chemical Shifts of Free-Base Porphyrinoids. <i>Chemistry</i> , 2021 , 3, 1005-1021	3.6	1