# Heike Fliegl

## List of Publications by Year in Descending Order



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|---|---|---|---|
| 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 | Determinant Factors of Three-Dimensional Aromaticity in Antiaromatic Cyclophanes. *Journal of the American Chemical Society*, **2021**, 143, 10676-10685 | 16.4 | 9 |
| 61 | Spatial Contributions to Nuclear Magnetic Shieldings. *Journal of Physical Chemistry A*, **2021**, 125, 1778-1786 | 2.8 | 8 |
| 60 | Benchmarking Magnetizabilities with Recent Density Functionals. *Journal of Chemical Theory and Computation*, **2021**, 17, 1457-1468 | 6.4 | 19 |
| 59 | Spatial Contributions to 1H NMR Chemical Shifts of Free-Base Porphyrinoids. *Chemistry*, **2021**, 3, 1005-1021 | 2.1 | 1 |
| 58 | The effect of anion complexation on the aromatic properties of aromatic and antiaromatic porphyrinoids. *New Journal of Chemistry*, **2020**, 44, 20643-20650 | 3.6 | 2 |
| 57 | Tacticity dependence of single chain polymer folding. *Polymer Chemistry*, **2020**, 11, 3439-3445 | 4.9 | 3 |
| 56 | Calculation of vibrationally resolved absorption spectra of acenes and pyrene. *Physical Chemistry Chemical Physics*, **2019**, 21, 21094-21103 | 3.6 | 26 |
| 55 | Four-component relativistic P NMR calculations for trans-platinum(ii) complexes: importance of the solvent and dynamics in spectral simulations. *Dalton Transactions*, **2019**, 48, 8076-8083 | 4.3 | 13 |
| 54 | Ni(II) 10-Phosphacorrole: A Porphyrin Analogue Containing Phosphorus at the Meso Position. *Journal of the American Chemical Society*, **2019**, 141, 4800-4805 | 16.4 | 17 |
| 53 | Absorption shifts of diastereotopically ligated chlorophyll dimers of photosystem I. *Physical Chemistry Chemical Physics*, **2019**, 21, 6851-6858 | 3.6 | 12 |
| 52 | Three-dimensional aromaticity in an antiaromatic cyclophane. *Nature Communications*, **2019**, 10, 3576 | 17.4 | 39 |
| 51 | Magnetically Induced Ring-Current Strengths in Möbius Twisted Annulenes. *Journal of Physical Chemistry Letters*, **2018**, 9, 1627-1632 | 6.4 | 11 |
| 50 | Rational Synthesis of Antiaromatic 5,15-Dioxaporphyrin and Oxidation into π-Linked Dimers. *Angewandte Chemie*, **2018**, 130, 9876-9881 | 3.6 | 7 |
| 49 | Accelerating Kohn-Sham response theory using density fitting and the auxiliary-density-matrix method. *International Journal of Quantum Chemistry*, **2018**, 118, e25639 | 2.1 | 8 |
| 48 | Computational Studies of Aromatic and Photophysical Properties of Expanded Porphyrins. *Journal of Physical Chemistry A*, **2018**, 122, 4756-4767 | 2.8 | 33 |
| 47 | Rational Synthesis of Antiaromatic 5,15-Dioxaporphyrin and Oxidation into π-Linked Dimers. *Angewandte Chemie - International Edition*, **2018**, 57, 9728-9733 | 16.4 | 23 |
| 46 | Bicycloaromaticity and Baird-type bicycloaromaticity of dithienothiophene-bridged [34]octaphyrins. *Physical Chemistry Chemical Physics*, **2018**, 20, 17705-17713 | 3.6 | 17 |

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| 45 | Aromaticity introduced by antiferromagnetic ligand mediated metal–metal interactions. Insights from the induced magnetic response in [Cu6(dmPz)6(OH)6]. *Inorganic Chemistry Frontiers*, **2017**, 4, 986-993 | 6.8 | 8 |
| 44 | Closed-shell paramagnetic porphyrinoids. *Chemical Communications*, **2017**, 53, 9866-9869 | 5.8 | 31 |
| 43 | Relation Between Ring Currents and Hydrogenation Enthalpies for Assessing the Degree of Aromaticity. *Journal of Physical Chemistry A*, **2017**, 121, 7282-7289 | 2.8 | 32 |
| 42 | Optical and magnetic properties of antiaromatic porphyrinoids. *Physical Chemistry Chemical Physics*, **2017**, 19, 25979-25988 | 3.6 | 17 |
| 41 | The influence of heteroatoms on the aromatic character and the current pathways of BN-dibenzo[a,e]pentalenes. *Physical Chemistry Chemical Physics*, **2017**, 19, 20213-20223 | 3.6 | 12 |
| 40 | Gauge-Origin Independent Calculations of the Anisotropy of the Magnetically Induced Current Densities. *Journal of Physical Chemistry A*, **2016**, 120, 5658-64 | 2.8 | 35 |
| 39 | Analysis of the magnetically induced current density of molecules consisting of annelated aromatic and antiaromatic hydrocarbon rings. *Physical Chemistry Chemical Physics*, **2016**, 18, 15934-42 | 3.6 | 43 |
| 38 | Evaluating Shielding-Based Ring-Current Models by Using the Gauge-Including Magnetically Induced Current Method. *Journal of the Chinese Chemical Society*, **2016**, 63, 93-100 | 1.5 | 14 |
| 37 | New insights into aromatic pathways of carbachlorins and carbaporphyrins based on calculations of magnetically induced current densities. *Physical Chemistry Chemical Physics*, **2016**, 18, 11932-41 | 3.6 | 26 |
| 36 | Calculations of magnetically induced current densities: theory and applications. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2016**, 6, 639-678 | 7.9 | 174 |
| 35 | Nuclei-selected atomic-orbital response-theory formulation for the calculation of NMR shielding tensors using density-fitting. *Journal of Chemical Physics*, **2016**, 145, 234108 | 3.9 | 6 |
| 34 | The Excitation Spectra of Naphthalene Dimers: Frenkel and Charge-transfer Excitons. *Journal of the Chinese Chemical Society*, **2016**, 63, 20-32 | 1.5 | 3 |
| 33 | Predicting the degree of aromaticity of novel carbaporphyrinoids. *Physical Chemistry Chemical Physics*, **2015**, 17, 14215-22 | 3.6 | 24 |
| 32 | Antiaromatic character of 16 π-electron octaethylporphyrins: magnetically induced ring currents from DFT-GIMIC calculations. *Journal of Physical Chemistry A*, **2015**, 119, 2344-50 | 2.8 | 23 |
| 31 | The origin dependence of the material constants: the permittivity and the inverse permeability. *Molecular Physics*, **2015**, 113, 1899-1913 | 1.7 | 6 |
| 30 | Aromatic pathways in carbathiaporphyrins. *Journal of Physical Chemistry A*, **2015**, 119, 1201-7 | 2.8 | 23 |
| 29 | The Dalton quantum chemistry program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 269-284 | 7.9 | 956 |
| 28 | Coupled-cluster calculations of the lowest 0-0 bands of the electronic excitation spectrum of naphthalene. *Physical Chemistry Chemical Physics*, **2014**, 16, 9859-65 | 3.6 | 14 |

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| 27 | Unusual formation of a N-heterocyclic germylene via homolytic cleavage of a C-C bond. *Chemical Communications*, **2014**, 50, 3356-8 | 5.8 | 21 |
| 26 | The aromatic character of thienopyrrole-modified 20π-electron porphyrinoids. *Physical Chemistry Chemical Physics*, **2014**, 16, 11010-6 | 3.6 | 25 |
| 25 | Mechanistic insights on the stereoselective nucleophilic 1,2-addition to sulfinyl imines. *Journal of Organic Chemistry*, **2014**, 79, 2514-21 | 4.2 | 16 |
| 24 | 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 | 3.6 | 4 |
| 23 | Insights into magnetically induced current pathways and optical properties of isophlorins. *Journal of Physical Chemistry A*, **2013**, 117, 9062-8 | 2.8 | 37 |
| 22 | Heteroaromaticity approached by charge density investigations and electronic structure calculations. *Physical Chemistry Chemical Physics*, **2013**, 15, 20600-10 | 3.6 | 27 |
| 21 | All-Metal Aromaticity: Revisiting the Ring Current Model among Transition Metal Clusters. *Journal of Chemical Theory and Computation*, **2013**, 9, 4789-96 | 6.4 | 75 |
| 20 | Non-perturbative treatment of molecules in linear magnetic fields: calculation of anapole susceptibilities. *Journal of Chemical Physics*, **2013**, 139, 164118 | 3.9 | 25 |
| 19 | 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 | 27 |
| 18 | Aromatic pathways of porphins, chlorins, and bacteriochlorins. *Journal of Organic Chemistry*, **2012**, 77, 3408-14 | 4.2 | 69 |
| 17 | Effect of fluorine substitution on the aromaticity of polycyclic hydrocarbons. *Journal of Physical Chemistry A*, **2012**, 116, 10257-68 | 2.8 | 50 |
| 16 | The gauge including magnetically induced current method. *Physical Chemistry Chemical Physics*, **2011**, 13, 20500-18 | 3.6 | 231 |
| 15 | Hydrogen-bond strengths by magnetically induced currents. *Physical Chemistry Chemical Physics*, **2011**, 13, 434-7 | 3.6 | 34 |
| 14 | Theoretical investigation of photoelectron spectra and magnetically induced current densities in ring-shaped transition-metal oxides. *Theoretical Chemistry Accounts*, **2011**, 129, 701-713 | 1.9 | 11 |
| 13 | Aromatic pathways in mono- and bisphosphorous singly Möbius twisted [28] and [30]hexaphyrins. *Physical Chemistry Chemical Physics*, **2011**, 13, 20659-65 | 3.6 | 37 |
| 12 | Aromatic pathways in twisted hexaphyrins. *Journal of Physical Chemistry A*, **2010**, 114, 7153-61 | 2.8 | 57 |
| 11 | 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, 10477-83 | 16.4 | 39 |
| 10 | Magnetically induced current densities in aromatic, antiaromatic, homoaromatic, and nonaromatic hydrocarbons. *Journal of Physical Chemistry A*, **2009**, 113, 8668-76 | 2.8 | 138 |

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| 9 | Expanding the coordination cage: a ruthenium(II)-polypyridine complex exhibiting high quantum yields under ambient conditions. *Inorganic Chemistry*, **2009**, 48, 5677-84 | 5.1 | 67 |
| 8 | 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. *Physical Chemistry Chemical Physics*, **2009**, 11, 3900-9 | 3.6 | 20 |
| 7 | Calculation of magnetically induced currents in hydrocarbon nanorings. *Journal of Physical Chemistry A*, **2008**, 112, 13584-92 | 2.8 | 32 |
| 6 | Accurate computational determination of the binding energy of the SO3 x H2O complex. *Journal of Chemical Physics*, **2006**, 125, 054312 | 3.9 | 26 |
| 5 | Coupled-cluster response theory with linear-r12 corrections: the CC2-R12 model for excitation energies. *Journal of Chemical Physics*, **2006**, 124, 044112 | 3.9 | 46 |
| 4 | 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 | 2.1 | 66 |
| 3 | Coupled-cluster theory with simplified linear-r(12) corrections: the CCSD(R12) model. *Journal of Chemical Physics*, **2005**, 122, 84107 | 3.9 | 158 |
| 2 | Ab initio calculation of the vibrational and electronic spectra of trans- and cis-azobenzene. *Journal of the American Chemical Society*, **2003**, 125, 9821-7 | 16.4 | 168 |
| 1 | Theoretical studies as a tool for understanding the aromatic character of porphyrinoid compounds. *Chemical Modelling*,1-42 | 2 | 25 |