Felix Plasser

List of Publications by Year
in descending order

99 papers	7,906 citations	81743 39 h-index	49773 87 g-index
124 all docs	124 docs citations	124 times ranked	6098 citing authors

#	Article	IF	Citations
1	Spin-density calculation via the graphical unitary group approach. Molecular Physics, 2023, 121, .	0.8	3
2	libwfa: Wavefunction analysis tools for excited and openâ€shell electronic states. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	6.2	16
3	Sterically demanding macrocyclic Eu(<scp>iii</scp>) complexes for selective recognition of phosphate and real-time monitoring of enzymatically generated adenosine monophosphate. Chemical Science, 2022, 13, 3386-3394.	3.7	14
4	Reversible Pâ€“P bond cleavage at an iridium(<scp>iii</scp>) metal centre. Chemical Communications, 2022, 58, 5598-5601.	2.2	3
5	Donorâ€“Acceptorâ€“Donor â€œHot Excitonâ€•Triads for High Reverse Intersystem Crossing in OLEDs. Advanced Optical Materials, 2022, 10, .	3.6	7
6	Oxygen harvesting from carbon dioxide: simultaneous epoxidation and CO formation. Chemical Science, 2021, 12, 13373-13378.	3.7	5
7	Excited-state symmetry breaking in 9,10-dicyanoanthracene-based quadrupolar molecules: the effect of donorâ€“acceptor branch length. Physical Chemistry Chemical Physics, 2021, 23, 15150-15158.	1.3	11
8	Identifying the Trade-off between Intramolecular Singlet Fission Requirements in Donorâ€“Acceptor Copolymers. Chemistry of Materials, 2021, 33, 2567-2575.	3.2	14
9	Elucidating the Electronic Structure of a Delayed Fluorescence Emitter via Orbital Interactions, Excitation Energy Components, Charge-Transfer Numbers, and Vibrational Reorganization Energies. Journal of Physical Chemistry Letters, 2021, 12, 2712-2720.	2.1	35
10	Mechanistic insight into the fluorescence activity of forensic fingerprinting reagents. Journal of Chemical Physics, 2021, 154, 124313.	1.2	3
11	Excited-state dynamics of [Mn(im)(CO)3(phen)]+: PhotoCORM, catalyst, luminescent probe?. Journal of Chemical Physics, 2021, 154, 154102.	1.2	8
12	Exploitation of Baird Aromaticity and Clarâ€™s Rule for Tuning the Triplet Energies of Polycyclic Aromatic Hydrocarbons. Chemistry, 2021, 3, 532-549.	0.9	15
13	Visualisation of Chemical Shielding Tensors (VIST) to Elucidate Aromaticity and Antiaromaticity**. European Journal of Organic Chemistry, 2021, 2021, 2529-2539.	1.2	16
14	Pushing the Limits of the Donorâ€“Acceptor Copolymer Strategy for Intramolecular Singlet Fission. Journal of Physical Chemistry Letters, 2021, 12, 7270-7277.	2.1	5
15	Highly sensitive 26Al measurements by Ion-Laser-InterAction Mass Spectrometry. International Journal of Mass Spectrometry, 2021, 465, 116576.	0.7	14
16	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
17	Surface Hopping Dynamics on Vibronic Coupling Models. Accounts of Chemical Research, 2021, 54, 3760-3771.	7.6	32
18	Functional group introduction and aromatic unit variation in a set of Ï€-conjugated macrocycles: revealing the central role of local and global aromaticity. Organic Chemistry Frontiers, 2021, 8, 4730-4745.	2.3	10

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19	The role of excited-state character, structural relaxation, and symmetry breaking in enabling delayed fluorescence activity in pushâ€“pull chromophores. Physical Chemistry Chemical Physics, 2021, 23, 26135-26150.	1.3	10
20	Designing Singlet Fission Candidates from Donorâ€“Acceptor Copolymers. Chemistry of Materials, 2020, 32, 6515-6524.	3.2	27
21	A complementary approach to conjugated N-acyliminium formation through photoredox-catalyzed intermolecular radical addition to allenamides and allencarbamates. Beilstein Journal of Organic Chemistry, 2020, 16, 1983-1990.	1.3	10
22	Annihilation Dynamics of Molecular Excitons Measured at a Single Perturbative Excitation Energy. Journal of Physical Chemistry Letters, 2020, 11, 7776-7781.	2.1	17
23	Optical absorption properties of metalâ€“organic frameworks: solid state versus molecular perspective. Physical Chemistry Chemical Physics, 2020, 22, 19512-19521.	1.3	14
24	Direct, Mediated, and Delayed Intramolecular Singlet Fission Mechanism in Donorâ€“Acceptor Copolymers. Journal of Physical Chemistry Letters, 2020, 11, 9788-9794.	2.1	11
25	Orbital-free photophysical descriptors to predict directional excitations in metal-based photosensitizers. Chemical Science, 2020, 11, 7685-7693.	3.7	9
26	Multiâ€Tier Electronic Structure Analysis of Sita's Mo and W Complexes Capable of Thermal or Photochemical N₂Splitting. European Journal of Inorganic Chemistry, 2020, 2020, 1506-1518.	1.0	10
27	Solution processed CZTS solar cells using amineâ€“thiol systems: understanding the dissolution process and device fabrication. Journal of Materials Chemistry C, 2020, 8, 10309-10318.	2.7	11
28	Toward an understanding of electronic excitation energies beyond the molecular orbital picture. Physical Chemistry Chemical Physics, 2020, 22, 6058-6080.	1.3	60
29	TheoDORE: A toolbox for a detailed and automated analysis of electronic excited state computations. Journal of Chemical Physics, 2020, 152, 084108.	1.2	209
30	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	1.2	42
31	A systematic analysis of excitonic properties to seek optimal singlet fission: the BN-substitution patterns in tetracene. Journal of Materials Chemistry C, 2020, 8, 7793-7804.	2.7	22
32	Strong Influence of Decoherence Corrections and Momentum Rescaling in Surface Hopping Dynamics of Transition Metal Complexes. Journal of Chemical Theory and Computation, 2019, 15, 5031-5045.	2.3	50
33	Computational Assessment of MLCT versus MC Stabilities in Firstâ€toâ€Thirdâ€Row d 6 Pseudoâ€Octahedral Transition Metal Complexes. Journal of Computational Chemistry, 2019, 40, 2377-2390.	1.5	4
34	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	2.3	661
35	Dynamics of benzene excimer formation from the parallel-displaced dimer. Physical Chemistry Chemical Physics, 2019, 21, 13916-13924.	1.3	23
36	Highly efficient surface hopping dynamics using a linear vibronic coupling model. Physical Chemistry Chemical Physics, 2019, 21, 57-69.	1.3	81

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37	Effect of symmetric and asymmetric substitution on the optoelectronic properties of 9,10-dicyanoanthracene. Molecular Systems Design and Engineering, 2019, 4, 951-961.	1.7	13
38	Red-shifted delayed fluorescence at the expense of photoluminescence quantum efficiency â€“ an intramolecular charge-transfer molecule based on a benzodithiophene-4,8-dione acceptor. Physical Chemistry Chemical Physics, 2019, 21, 10580-10586.	1.3	11
39	The Influence of the Electronic Structure Method on Intersystem Crossing Dynamics. The Case of Thioformaldehyde. Journal of Chemical Theory and Computation, 2019, 15, 3470-3480.	2.3	30
40	Visualisation of Electronic Excitedâ€State Correlation in Real Space. ChemPhotoChem, 2019, 3, 702-706.	1.5	16
41	Excitedâ€State Reactivity of [Mn(im)(CO)₃(phen)]⁺: A Structural Exploration. Journal of Computational Chemistry, 2019, 40, 72-81.	1.5	7
42	Quantitative wave function analysis for excited states of transition metal complexes. Coordination Chemistry Reviews, 2018, 361, 74-97.	9.5	109
43	Benchmarking Excited-State Calculations Using Exciton Properties. Journal of Chemical Theory and Computation, 2018, 14, 710-725.	2.3	128
44	Interstate vibronic coupling constants between electronic excited states for complex molecules. Journal of Chemical Physics, 2018, 148, 124119.	1.2	33
45	Wavelength-optimized Two-Photon Polymerization Using Initiators Based on Multipolar Aminostyryl-1,3,5-triazines. Scientific Reports, 2018, 8, 17273.	1.6	32
46	Surface Hopping within an Exciton Picture. An Electrostatic Embedding Scheme. Journal of Chemical Theory and Computation, 2018, 14, 6139-6148.	2.3	29
47	Multireference Approaches for Excited States of Molecules. Chemical Reviews, 2018, 118, 7293-7361.	23.0	287
48	Ultrafast Intersystem Crossing vs Internal Conversion in Î±-Diimine Transition Metal Complexes: Quantum Evidence. Journal of Physical Chemistry Letters, 2018, 9, 5189-5195.	2.1	30
49	Ultrafast Electronic Energy Transfer in an Orthogonal Molecular Dyad. Journal of Physical Chemistry Letters, 2017, 8, 1086-1092.	2.1	32
50	Universal Exciton Size in Organic Polymers is Determined by Nonlocal Orbital Exchange in Time-Dependent Density Functional Theory. Journal of Physical Chemistry Letters, 2017, 8, 1205-1210.	2.1	49
51	Ultrafast Excited-State Decays in [Re(CO)₃(N,N)(L)]ⁿ⁺: Nonadiabatic Quantum Dynamics. Journal of Chemical Theory and Computation, 2017, 13, 1293-1306.	2.3	45
52	UV absorption in metal decorated boron nitride flakes: a theoretical analysis of excited states. Molecular Physics, 2017, 115, 2469-2477.	0.8	5
53	Local Electron Correlation Treatment in Extended Multireference Calculations: Effect of Acceptorâ€“Donor Substituents on the Biradical Character of the Polycyclic Aromatic Hydrocarbon Heptazethrene. Journal of Chemical Theory and Computation, 2017, 13, 2612-2622.	2.3	13
54	Electronic delocalization, charge transfer and hypochromism in the UV absorption spectrum of polyadenine unravelled by multiscale computations and quantitative wavefunction analysis. Chemical Science, 2017, 8, 5682-5691.	3.7	79

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55	Evaluation of the quasi correlated tight-binding (QCTB) model for describing polyradical character in polycyclic hydrocarbons. Journal of Chemical Physics, 2017, 146, 064106.	1.2	21
56	Color Fineâ€Tuning of Optical Materials Through Rational Design. ChemPhysChem, 2017, 18, 549-563.	1.0	15
57	Excited-states of a rhenium carbonyl diimine complex: solvation models, spinâ€“orbit coupling, and vibrational sampling effects. Physical Chemistry Chemical Physics, 2017, 19, 27240-27250.	1.3	40
58	Detailed Wave Function Analysis for Multireference Methods: Implementation in the <scp>Molcas</scp> Program Package and Applications to Tetracene. Journal of Chemical Theory and Computation, 2017, 13, 5343-5353.	2.3	40
59	Chromophores from hexeneuronic acids: identification of HexA-derived chromophores. Cellulose, 2017, 24, 3671-3687.	2.4	23
60	Surface hopping dynamics including intersystem crossing using the algebraic diagrammatic construction method. Journal of Chemical Physics, 2017, 147, 184109.	1.2	32
61	Nonadiabatic Dynamics of Cycloparaphenylenes with TD-DFTB Surface Hopping. Journal of Chemical Theory and Computation, 2017, 13, 5846-5860.	2.3	46
62	Charge-transfer states in triazole linked donorâ€“acceptor materials: strong effects of chemical modification and solvation. Physical Chemistry Chemical Physics, 2017, 19, 18055-18067.	1.3	19
63	Challenges in Simulating Light-Induced Processes in DNA. Molecules, 2017, 22, 49.	1.7	21
64	Entanglement entropy of electronic excitations. Journal of Chemical Physics, 2016, 144, 194107.	1.2	44
65	Communication: Unambiguous comparison of many-electron wavefunctions through their overlaps. Journal of Chemical Physics, 2016, 145, 021103.	1.2	19
66	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. Journal of Computational Chemistry, 2016, 37, 506-541.	1.5	1,317
67	Electronic and Photophysical Properties of [Re (L)(CO)₃(phen)]⁺ and [Ru(L)₂(bpy)₂]²⁺ (L = imidazole), Building Units for Long-Range Electron Transfer in Modified Blue Copper Proteins. Journal of Physical Chemistry A, 2016, 120, 6934-6943.	1.1	17
68	Description of excited states in [Re(Imidazole)(CO)₃(Phen)]⁺ including solvent and spinâ€orbit coupling effects: Density functional theory versus multiconfigurational wavefunction approach. Journal of Computational Chemistry, 2016, 37, 2454-2466.	1.5	30
69	Excitons in poly(para phenylene vinylene): a quantum-chemical perspective based on high-level ab initio calculations. Physical Chemistry Chemical Physics, 2016, 18, 2548-2563.	1.3	57
70	Polyradical Character of Triangular Non-KekulÃ© Structures, Zethrenes, p-Quinodimethane-Linked Bisphenalenyl, and the Clar Goblet in Comparison: An Extended Multireference Study. Journal of Physical Chemistry A, 2016, 120, 1625-1636.	1.1	91
71	Efficient and Flexible Computation of Many-Electron Wave Function Overlaps. Journal of Chemical Theory and Computation, 2016, 12, 1207-1219.	2.3	145
72	Exciton size and binding energy limitations in one-dimensional organic materials. Journal of Chemical Physics, 2015, 143, 244905.	1.2	59

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73	Communication: Exciton analysis in time-dependent density functional theory: How functionals shape excited-state characters. Journal of Chemical Physics, 2015, 143, 171101.	1.2	74
74	Statistical analysis of electronic excitation processes: Spatial location, compactness, charge transfer, and electron-hole correlation. Journal of Computational Chemistry, 2015, 36, 1609-1620.	1.5	95
75	Intramolecular Charge-Transfer Excited-State Processes in 4-(N,N-Dimethylamino)benzonitrile: The Role of Twisting and the ï€ï*f* State. Journal of Physical Chemistry A, 2015, 119, 6232-6243.	1.1	60
76	High-Level Ab Initio Computations of the Absorption Spectra of Organic Iridium Complexes. Journal of Physical Chemistry A, 2015, 119, 1023-1036.	1.1	34
77	Exciton analysis of many-body wave functions: Bridging the gap between the quasiparticle and molecular orbital pictures. Physical Review A, 2014, 90, .	1.0	131
78	Study of the Diradicaloid Character in a Prototypical Pancakeâ€Bonded Dimer: The Stacked Tetracyanoethylene (TCNE) Anion Dimer and the Neutral K₂TCNE₂ Complex. ChemPhysChem, 2014, 15, 165-176.	1.0	43
79	Perturbational treatment of spin-orbit coupling for generally applicable high-level multi-reference methods. Journal of Chemical Physics, 2014, 141, 074105.	1.2	33
80	New tools for the systematic analysis and visualization of electronic excitations. I. Formalism. Journal of Chemical Physics, 2014, 141, 024106.	1.2	369
81	New tools for the systematic analysis and visualization of electronic excitations. II. Applications. Journal of Chemical Physics, 2014, 141, 024107.	1.2	199
82	Electronic Excitation Processes in Single-Strand and Double-Strand DNA: A Computational Approach. Topics in Current Chemistry, 2014, 356, 1-37.	4.0	20
83	Surface Hopping Dynamics with Correlated Single-Reference Methods: 9H-Adenine as a Case Study. Journal of Chemical Theory and Computation, 2014, 10, 1395-1405.	2.3	170
84	A comparison of singlet and triplet states for one- and two-dimensional graphene nanoribbons using multireference theory. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	56
85	Newtonâ€<scp>X</scp>: a surfaceâ€hopping program for nonadiabatic molecular dynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 26-33.	6.2	370
86	Electronic excitation and structural relaxation of the adenine dinucleotide in gas phase and solution. Photochemical and Photobiological Sciences, 2013, 12, 1440-1452.	1.6	46
87	The Multiradical Character of Oneâ€and Twoâ€Dimensional Graphene Nanoribbons. Angewandte Chemie - International Edition, 2013, 52, 2581-2584.	7.2	197
88	Synthesis, Spectroscopy, and Computational Analysis of Photoluminescent Bis(aminophenyl)â€Substituted Thiophene Derivatives. ChemPhysChem, 2013, 14, 1016-1024.	1.0	18
89	Electronically Excited States in Poly(p-phenylenevinylene): Vertical Excitations and Torsional Potentials from High-Level Ab Initio Calculations. Journal of Physical Chemistry A, 2013, 117, 2181-2189.	1.1	65
90	Surface hopping dynamics using a locally diabatic formalism: Charge transfer in the ethylene dimer cation and excited state dynamics in the 2-pyridone dimer. Journal of Chemical Physics, 2012, 137, 22A514.	1.2	173

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91	Analysis of Excitonic and Charge Transfer Interactions from Quantum Chemical Calculations. Journal of Chemical Theory and Computation, 2012, 8, 2777-2789.	2.3	375
92	UV Absorption Spectrum of Alternating DNA Duplexes. Analysis of Excitonic and Charge Transfer Interactions. Journal of Physical Chemistry A, 2012, 116, 11151-11160.	1.1	70
93	The effect of hydrogen bonding on the excited-state proton transfer in 2-(2â€²-hydroxyphenyl)benzothiazole: a TDDFT molecular dynamics study. Physical Chemistry Chemical Physics, 2012, 14, 9016.	1.3	69
94	Electronically excited states and photodynamics: a continuing challenge. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	77
95	Electronically excited states and photodynamics: a continuing challenge. , 2012, , 147-160.		1
96	Semiclassical dynamics simulations of charge transport in stacked Ï€-systems. Journal of Chemical Physics, 2011, 134, 034309.	1.2	27
97	Excited-State Diproton Transfer in [2,2â€²-Bipyridyl]-3,3â€²-diol: the Mechanism Is Sequential, Not Concerted. Journal of Physical Chemistry A, 2009, 113, 8490-8499.	1.1	110
98	[2.2.2.2]Paracyclophanetetraenes (PCTs): cyclic structural analogues of poly(pâ€˜phenylene vinylene)s (PPVs). Open Research Europe, 0, 1, 111.	2.0	2
99	[2.2.2.2]Paracyclophanetetraenes (PCTs): cyclic structural analogues of poly(pâ€˜phenylene vinylene)s (PPVs). Open Research Europe, 0, 1, 111.	2.0	4