

Felix Plasser

List of Publications by Year in descending order

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99
papers

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81743

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87
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124
all docs

124
docs citations

124
times ranked

6098
citing authors

#	ARTICLE	IF	CITATIONS
1	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. <i>Journal of Computational Chemistry</i> , 2016, 37, 506-541.	1.5	1,317
2	OpenMolcas: From Source Code to Insight. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5925-5964.	2.3	661
3	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	1.2	518
4	Analysis of Excitonic and Charge Transfer Interactions from Quantum Chemical Calculations. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2777-2789.	2.3	375
5	Newtonâ€‹X</scp>: a surfaceâ€‹hopping program for nonadiabatic molecular dynamics. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2014, 4, 26-33.	6.2	370
6	New tools for the systematic analysis and visualization of electronic excitations. I. Formalism. <i>Journal of Chemical Physics</i> , 2014, 141, 024106.	1.2	369
7	Multireference Approaches for Excited States of Molecules. <i>Chemical Reviews</i> , 2018, 118, 7293-7361.	23.0	287
8	TheoDORE: A toolbox for a detailed and automated analysis of electronic excited state computations. <i>Journal of Chemical Physics</i> , 2020, 152, 084108.	1.2	209
9	New tools for the systematic analysis and visualization of electronic excitations. II. Applications. <i>Journal of Chemical Physics</i> , 2014, 141, 024107.	1.2	199
10	The Multiradical Character of Oneâ€‹and Twoâ€‹Dimensional Graphene Nanoribbons. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 2581-2584.	7.2	197
11	Surface hopping dynamics using a locally diabatic formalism: Charge transfer in the ethylene dimer cation and excited state dynamics in the 2-pyridone dimer. <i>Journal of Chemical Physics</i> , 2012, 137, 22A514.	1.2	173
12	Surface Hopping Dynamics with Correlated Single-Reference Methods: 9H-Adenine as a Case Study. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1395-1405.	2.3	170
13	Efficient and Flexible Computation of Many-Electron Wave Function Overlaps. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1207-1219.	2.3	145
14	Exciton analysis of many-body wave functions: Bridging the gap between the quasiparticle and molecular orbital pictures. <i>Physical Review A</i> , 2014, 90, .	1.0	131
15	Benchmarking Excited-State Calculations Using Exciton Properties. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 710-725.	2.3	128
16	Excited-State Diproton Transfer in [2,2â€‹-Bipyridyl]-3,3â€‹-diol: the Mechanism Is Sequential, Not Concerted. <i>Journal of Physical Chemistry A</i> , 2009, 113, 8490-8499.	1.1	110
17	Quantitative wave function analysis for excited states of transition metal complexes. <i>Coordination Chemistry Reviews</i> , 2018, 361, 74-97.	9.5	109
18	Statistical analysis of electronic excitation processes: Spatial location, compactness, charge transfer, and electron-hole correlation. <i>Journal of Computational Chemistry</i> , 2015, 36, 1609-1620.	1.5	95

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19	Polyradical Character of Triangular Non-Kekulé Structures, Zethrenes, <i>p</i> -Quinodimethane-Linked Bisphenalenyl, and the Clar Goblet in Comparison: An Extended Multireference Study. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1625-1636.	1.1	91
20	Highly efficient surface hopping dynamics using a linear vibronic coupling model. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 57-69.	1.3	81
21	Electronic delocalization, charge transfer and hypochromism in the UV absorption spectrum of polyadenine unravelled by multiscale computations and quantitative wavefunction analysis. <i>Chemical Science</i> , 2017, 8, 5682-5691.	3.7	79
22	Electronically excited states and photodynamics: a continuing challenge. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	77
23	Communication: Exciton analysis in time-dependent density functional theory: How functionals shape excited-state characters. <i>Journal of Chemical Physics</i> , 2015, 143, 171101.	1.2	74
24	UV Absorption Spectrum of Alternating DNA Duplexes. Analysis of Excitonic and Charge Transfer Interactions. <i>Journal of Physical Chemistry A</i> , 2012, 116, 11151-11160.	1.1	70
25	The effect of hydrogen bonding on the excited-state proton transfer in 2-(2-hydroxyphenyl)benzothiazole: a TDDFT molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 9016.	1.3	69
26	Electronically Excited States in Poly(<i>p</i> -phenylenevinylene): Vertical Excitations and Torsional Potentials from High-Level Ab Initio Calculations. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2181-2189.	1.1	65
27	Intramolecular Charge-Transfer Excited-State Processes in 4-(<i>N,N</i> -Dimethylamino)benzonitrile: The Role of Twisting and the π^* State. <i>Journal of Physical Chemistry A</i> , 2015, 119, 6232-6243.	1.1	60
28	Toward an understanding of electronic excitation energies beyond the molecular orbital picture. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 6058-6080.	1.3	60
29	Exciton size and binding energy limitations in one-dimensional organic materials. <i>Journal of Chemical Physics</i> , 2015, 143, 244905.	1.2	59
30	Excitons in poly(<i>para</i> phenylene vinylene): a quantum-chemical perspective based on high-level ab initio calculations. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 2548-2563.	1.3	57
31	A comparison of singlet and triplet states for one- and two-dimensional graphene nanoribbons using multireference theory. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	56
32	Strong Influence of Decoherence Corrections and Momentum Rescaling in Surface Hopping Dynamics of Transition Metal Complexes. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5031-5045.	2.3	50
33	Universal Exciton Size in Organic Polymers is Determined by Nonlocal Orbital Exchange in Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 1205-1210.	2.1	49
34	Electronic excitation and structural relaxation of the adenine dinucleotide in gas phase and solution. <i>Photochemical and Photobiological Sciences</i> , 2013, 12, 1440-1452.	1.6	46
35	Nonadiabatic Dynamics of Cycloparaphenylenes with TD-DFTB Surface Hopping. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5846-5860.	2.3	46
36	Ultrafast Excited-State Decays in $[\text{Re}(\text{CO})_3(\text{N},\text{N})(\text{L})]^{n+}$: Nonadiabatic Quantum Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1293-1306.	2.3	45

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37	Entanglement entropy of electronic excitations. <i>Journal of Chemical Physics</i> , 2016, 144, 194107.	1.2	44
38	Study of the Diradicaloid Character in a Prototypical Pancake- π -Bonded Dimer: The Stacked Tetracyanoethylene (TCNE) Anion Dimer and the Neutral K_2 -TCNE Complex. <i>ChemPhysChem</i> , 2014, 15, 165-176.	1.0	43
39	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. <i>Journal of Chemical Physics</i> , 2020, 152, 134110.	1.2	42
40	Excited-states of a rhenium carbonyl diimine complex: solvation models, spin-orbit coupling, and vibrational sampling effects. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 27240-27250.	1.3	40
41	Detailed Wave Function Analysis for Multireference Methods: Implementation in the Molcas Program Package and Applications to Tetracene. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5343-5353.	2.3	40
42	Elucidating the Electronic Structure of a Delayed Fluorescence Emitter via Orbital Interactions, Excitation Energy Components, Charge-Transfer Numbers, and Vibrational Reorganization Energies. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2712-2720.	2.1	35
43	High-Level Ab Initio Computations of the Absorption Spectra of Organic Iridium Complexes. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1023-1036.	1.1	34
44	Perturbational treatment of spin-orbit coupling for generally applicable high-level multi-reference methods. <i>Journal of Chemical Physics</i> , 2014, 141, 074105.	1.2	33
45	Interstate vibronic coupling constants between electronic excited states for complex molecules. <i>Journal of Chemical Physics</i> , 2018, 148, 124119.	1.2	33
46	Ultrafast Electronic Energy Transfer in an Orthogonal Molecular Dyad. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 1086-1092.	2.1	32
47	Surface hopping dynamics including intersystem crossing using the algebraic diagrammatic construction method. <i>Journal of Chemical Physics</i> , 2017, 147, 184109.	1.2	32
48	Wavelength-optimized Two-Photon Polymerization Using Initiators Based on Multipolar Aminostyryl-1,3,5-triazines. <i>Scientific Reports</i> , 2018, 8, 17273.	1.6	32
49	Surface Hopping Dynamics on Vibronic Coupling Models. <i>Accounts of Chemical Research</i> , 2021, 54, 3760-3771.	7.6	32
50	Description of excited states in $[Re(\text{Imidazole})(CO)_3(\text{Phen})]^{+}$ including solvent and spin-orbit coupling effects: Density functional theory versus multiconfigurational wavefunction approach. <i>Journal of Computational Chemistry</i> , 2016, 37, 2454-2466.	1.5	30
51	Ultrafast Intersystem Crossing vs Internal Conversion in $\hat{\pi}$ -Diimine Transition Metal Complexes: Quantum Evidence. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 5189-5195.	2.1	30
52	The Influence of the Electronic Structure Method on Intersystem Crossing Dynamics. The Case of Thioformaldehyde. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3470-3480.	2.3	30
53	Surface Hopping within an Exciton Picture. An Electrostatic Embedding Scheme. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 6139-6148.	2.3	29
54	Semiclassical dynamics simulations of charge transport in stacked π -systems. <i>Journal of Chemical Physics</i> , 2011, 134, 034309.	1.2	27

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55	Designing Singlet Fission Candidates from Donor–Acceptor Copolymers. <i>Chemistry of Materials</i> , 2020, 32, 6515-6524.	3.2	27
56	Chromophores from hexeneuronic acids: identification of HexA-derived chromophores. <i>Cellulose</i> , 2017, 24, 3671-3687.	2.4	23
57	Dynamics of benzene excimer formation from the parallel-displaced dimer. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 13916-13924.	1.3	23
58	A systematic analysis of excitonic properties to seek optimal singlet fission: the BN-substitution patterns in tetracene. <i>Journal of Materials Chemistry C</i> , 2020, 8, 7793-7804.	2.7	22
59	Evaluation of the quasi correlated tight-binding (QCTB) model for describing polyradical character in polycyclic hydrocarbons. <i>Journal of Chemical Physics</i> , 2017, 146, 064106.	1.2	21
60	Challenges in Simulating Light-Induced Processes in DNA. <i>Molecules</i> , 2017, 22, 49.	1.7	21
61	Electronic Excitation Processes in Single-Strand and Double-Strand DNA: A Computational Approach. <i>Topics in Current Chemistry</i> , 2014, 356, 1-37.	4.0	20
62	Communication: Unambiguous comparison of many-electron wavefunctions through their overlaps. <i>Journal of Chemical Physics</i> , 2016, 145, 021103.	1.2	19
63	Charge-transfer states in triazole linked donor–acceptor materials: strong effects of chemical modification and solvation. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 18055-18067.	1.3	19
64	Synthesis, Spectroscopy, and Computational Analysis of Photoluminescent Bis(aminophenyl)–Substituted Thiophene Derivatives. <i>ChemPhysChem</i> , 2013, 14, 1016-1024.	1.0	18
65	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. <i>Journal of Physical Chemistry A</i> , 2016, 120, 6934-6943.	1.1	17
66	Annihilation Dynamics of Molecular Excitons Measured at a Single Perturbative Excitation Energy. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 7776-7781.	2.1	17
67	Visualisation of Electronic Excited-State Correlation in Real Space. <i>ChemPhotoChem</i> , 2019, 3, 702-706.	1.5	16
68	Visualisation of Chemical Shielding Tensors (VIST) to Elucidate Aromaticity and Antiaromaticity**. <i>European Journal of Organic Chemistry</i> , 2021, 2021, 2529-2539.	1.2	16
69	libwfa: Wavefunction analysis tools for excited and open-shell electronic states. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2022, 12, .	6.2	16
70	Color Fine-Tuning of Optical Materials Through Rational Design. <i>ChemPhysChem</i> , 2017, 18, 549-563.	1.0	15
71	Exploitation of Baird Aromaticity and Clar's Rule for Tuning the Triplet Energies of Polycyclic Aromatic Hydrocarbons. <i>Chemistry</i> , 2021, 3, 532-549.	0.9	15
72	Optical absorption properties of metal–organic frameworks: solid state versus molecular perspective. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 19512-19521.	1.3	14

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73	Identifying the Trade-off between Intramolecular Singlet Fission Requirements in Donor–Acceptor Copolymers. <i>Chemistry of Materials</i> , 2021, 33, 2567-2575.	3.2	14
74	Highly sensitive ²⁶ Al measurements by Ion-Laser-InterAction Mass Spectrometry. <i>International Journal of Mass Spectrometry</i> , 2021, 465, 116576.	0.7	14
75	Sterically demanding macrocyclic Eu(III) complexes for selective recognition of phosphate and real-time monitoring of enzymatically generated adenosine monophosphate. <i>Chemical Science</i> , 2022, 13, 3386-3394.	3.7	14
76	Local Electron Correlation Treatment in Extended Multireference Calculations: Effect of Acceptor–Donor Substituents on the Biradical Character of the Polycyclic Aromatic Hydrocarbon Heptazethrene. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2612-2622.	2.3	13
77	Effect of symmetric and asymmetric substitution on the optoelectronic properties of 9,10-dicyanoanthracene. <i>Molecular Systems Design and Engineering</i> , 2019, 4, 951-961.	1.7	13
78	Red-shifted delayed fluorescence at the expense of photoluminescence quantum efficiency in an intramolecular charge-transfer molecule based on a benzodithiophene-4,8-dione acceptor. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 10580-10586.	1.3	11
79	Direct, Mediated, and Delayed Intramolecular Singlet Fission Mechanism in Donor–Acceptor Copolymers. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 9788-9794.	2.1	11
80	Solution processed CZTS solar cells using amine–thiol systems: understanding the dissolution process and device fabrication. <i>Journal of Materials Chemistry C</i> , 2020, 8, 10309-10318.	2.7	11
81	Excited-state symmetry breaking in 9,10-dicyanoanthracene-based quadrupolar molecules: the effect of donor–acceptor branch length. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15150-15158.	1.3	11
82	A complementary approach to conjugated <i>N</i> -acyliminium formation through photoredox-catalyzed intermolecular radical addition to allenamides and allencarbamates. <i>Beilstein Journal of Organic Chemistry</i> , 2020, 16, 1983-1990.	1.3	10
83	Multitier Electronic Structure Analysis of Sita's Mo and W Complexes Capable of Thermal or Photochemical N ₂ Splitting. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 1506-1518.	1.0	10
84	Functional group introduction and aromatic unit variation in a set of π-conjugated macrocycles: revealing the central role of local and global aromaticity. <i>Organic Chemistry Frontiers</i> , 2021, 8, 4730-4745.	2.3	10
85	The role of excited-state character, structural relaxation, and symmetry breaking in enabling delayed fluorescence activity in push–pull chromophores. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 26135-26150.	1.3	10
86	Orbital-free photophysical descriptors to predict directional excitations in metal-based photosensitizers. <i>Chemical Science</i> , 2020, 11, 7685-7693.	3.7	9
87	Excited-state dynamics of [Mn(III)(CO) ₃ (phen)] ⁺ : PhotoCORM, catalyst, luminescent probe?. <i>Journal of Chemical Physics</i> , 2021, 154, 154102.	1.2	8
88	Excited-State Reactivity of [Mn(III)(CO) ₃ (phen)] ⁺ : A Structural Exploration. <i>Journal of Computational Chemistry</i> , 2019, 40, 72-81.	1.5	7
89	Donor–Acceptor–Donor Hot Exciton–Triads for High Reverse Intersystem Crossing in OLEDs. <i>Advanced Optical Materials</i> , 2022, 10, .	3.6	7
90	UV absorption in metal decorated boron nitride flakes: a theoretical analysis of excited states. <i>Molecular Physics</i> , 2017, 115, 2469-2477.	0.8	5

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91	Oxygen harvesting from carbon dioxide: simultaneous epoxidation and CO formation. <i>Chemical Science</i> , 2021, 12, 13373-13378.	3.7	5
92	Pushing the Limits of the Donor–Acceptor Copolymer Strategy for Intramolecular Singlet Fission. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 7270-7277.	2.1	5
93	Computational Assessment of MLCT versus MC Stabilities in First-Row d 6 Pseudo-Octahedral Transition Metal Complexes. <i>Journal of Computational Chemistry</i> , 2019, 40, 2377-2390.	1.5	4
94	[2.2.2.2]Paracyclophanetetraenes (PCTs): cyclic structural analogues of poly(p-phenylene vinylene)s (PPVs). <i>Open Research Europe</i> , 0, 1, 111.	2.0	4
95	Mechanistic insight into the fluorescence activity of forensic fingerprinting reagents. <i>Journal of Chemical Physics</i> , 2021, 154, 124313.	1.2	3
96	Reversible P–P bond cleavage at an iridium(III) metal centre. <i>Chemical Communications</i> , 2022, 58, 5598-5601.	2.2	3
97	Spin-density calculation via the graphical unitary group approach. <i>Molecular Physics</i> , 2023, 121, .	0.8	3
98	[2.2.2.2]Paracyclophanetetraenes (PCTs): cyclic structural analogues of poly(p-phenylene vinylene)s (PPVs). <i>Open Research Europe</i> , 0, 1, 111.	2.0	2
99	Electronically excited states and photodynamics: a continuing challenge. , 2012, , 147-160.		1