Sebastian Mai

List of Publications by Year
in descending order

115 papers	8,714 citations	57758 44 h-index	43889 91 g-index
120 all docs	120 docs citations	120 times ranked	6313 citing authors

#	Article	IF	Citations
1	Spin-density calculation via the graphical unitary group approach. Molecular Physics, 2023, 121, .	1.7	3
2	libwfa: Wavefunction analysis tools for excited and openâ€shell electronic states. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	14.6	16
3	Reversible Pâ€“P bond cleavage at an iridium(<scp>iii</scp>) metal centre. Chemical Communications, 2022, 58, 5598-5601.	4.1	3
4	Ultrafast Intersystem Crossing Dynamics of 6-Selenoguanine in Water. Jacs Au, 2022, 2, 1699-1711.	7.9	10
5	Resolving Femtosecond Solvent Reorganization Dynamics in an Iron Complex by Nonadiabatic Dynamics Simulations. Journal of the American Chemical Society, 2022, 144, 12861-12873.	13.7	11
6	Oxygen harvesting from carbon dioxide: simultaneous epoxidation and CO formation. Chemical Science, 2021, 12, 13373-13378.	7.4	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.	2.8	11
8	Excited-State Properties and Relaxation Pathways of Selenium-Substituted Guanine Nucleobase in Aqueous Solution and DNA Duplex. Journal of Physical Chemistry B, 2021, 125, 1778-1789.	2.6	18
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.	4.6	35
10	A Force Field for a Manganese-Vanadium Water Oxidation Catalyst: Redox Potentials in Solution as Showcase. Catalysts, 2021, 11, 493.	3.5	8
11	Exploitation of Baird Aromaticity and Clarâ€™s Rule for Tuning the Triplet Energies of Polycyclic Aromatic Hydrocarbons. Chemistry, 2021, 3, 532-549.	2.2	15
12	Spectral Signatures of Oxidation States in a Manganeseâ€Oxo Cubane Water Oxidation Catalyst. Chemistry - A European Journal, 2021, 27, 17078-17086.	3.3	4
13	Surface Hopping Dynamics on Vibronic Coupling Models. Accounts of Chemical Research, 2021, 54, 3760-3771.	15.6	32
14	On the population of triplet states of 2-seleno-thymine. Physical Chemistry Chemical Physics, 2021, 23, 5447-5454.	2.8	7
15	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.	4.5	10
16	Jahnâ€Teller Effects in a Vanadateâ€Stabilized Manganeseâ€Oxo Cubane Water Oxidation Catalyst. Chemistry - A European Journal, 2021, 27, 17066-17077.	3.3	8
17	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.	2.8	10
18	Revealing Ultrafast Population Transfer between Nearly Degenerate Electronic States. Journal of Physical Chemistry Letters, 2020, 11, 1443-1449.	4.6	5

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19	Excimer Intermediates en Route to Long-Lived Charge-Transfer States in Single-Stranded Adenine DNA as Revealed by Nonadiabatic Dynamics. Journal of Physical Chemistry Letters, 2020, 11, 7483-7488.	4.6	21
20	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.	2.2	10
21	Implementation of Coherent Switching with Decay of Mixing into the SHARC Program. Journal of Chemical Theory and Computation, 2020, 16, 3464-3475.	5.3	18
22	Orbital-free photophysical descriptors to predict directional excitations in metal-based photosensitizers. Chemical Science, 2020, 11, 7685-7693.	7.4	9
23	Competing ultrafast photoinduced electron transfer and intersystem crossing of [Re(CO)$$_3$$(Dmp)(His124)(Trp122)]$$^+$$ in Pseudomonas aeruginosa azurin: a nonadiabatic dynamics study. Theoretical Chemistry Accounts, 2020, 139, 65.	1.4	17
24	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.	2.0	10
25	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.	5.5	11
26	Toward an understanding of electronic excitation energies beyond the molecular orbital picture. Physical Chemistry Chemical Physics, 2020, 22, 6058-6080.	2.8	60
27	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	3.0	42
28	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.	5.5	22
29	Molecular Photochemistry: Recent Developments in Theory. Angewandte Chemie - International Edition, 2020, 59, 16832-16846.	13.8	91
30	Molekulare Photochemie: Moderne Entwicklungen in der theoretischen Chemie. Angewandte Chemie, 2020, 132, 16976-16992.	2.0	1
31	Investigation of Complex Relaxation Dynamics of Nearly Degenerated Rydberg States in Acetone. , 2020, , .		0
32	Machine learning enables long time scale molecular photodynamics simulations. Chemical Science, 2019, 10, 8100-8107.	7.4	140
33	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.	5.3	50
34	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
35	Dynamics of benzene excimer formation from the parallel-displaced dimer. Physical Chemistry Chemical Physics, 2019, 21, 13916-13924.	2.8	23
36	Highly efficient surface hopping dynamics using a linear vibronic coupling model. Physical Chemistry Chemical Physics, 2019, 21, 57-69.	2.8	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.	3.4	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.	2.8	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.	5.3	30
40	Curious Case of 2-Selenouracil: Efficient Population of Triplet States and Yet Photostable. Journal of Chemical Theory and Computation, 2019, 15, 3730-3742.	5.3	14
41	Visualisation of Electronic Excitedâ€State Correlation in Real Space. ChemPhotoChem, 2019, 3, 702-706.	3.0	16
42	Unconventional two-step spin relaxation dynamics of [Re(CO)₃(im)(phen)]⁺ in aqueous solution. Chemical Science, 2019, 10, 10405-10411.	7.4	35
43	Identification of important normal modes in nonadiabatic dynamics simulations by coherence, correlation, and frequency analyses. Journal of Chemical Physics, 2019, 151, 244115.	3.0	16
44	Quantitative wave function analysis for excited states of transition metal complexes. Coordination Chemistry Reviews, 2018, 361, 74-97.	18.8	109
45	Benchmarking Excited-State Calculations Using Exciton Properties. Journal of Chemical Theory and Computation, 2018, 14, 710-725.	5.3	128
46	Interstate vibronic coupling constants between electronic excited states for complex molecules. Journal of Chemical Physics, 2018, 148, 124119.	3.0	33
47	Novel Molecular-Dynamics-Based Protocols for Phase Space Sampling in Complex Systems. Frontiers in Chemistry, 2018, 6, 495.	3.6	28
48	Wavelength-optimized Two-Photon Polymerization Using Initiators Based on Multipolar Aminostyryl-1,3,5-triazines. Scientific Reports, 2018, 8, 17273.	3.3	32
49	Surface Hopping within an Exciton Picture. An Electrostatic Embedding Scheme. Journal of Chemical Theory and Computation, 2018, 14, 6139-6148.	5.3	29
50	Simulated and Experimental Time-Resolved Photoelectron Spectra of the Intersystem Crossing Dynamics in 2-Thiouracil. Molecules, 2018, 23, 2836.	3.8	28
51	Cover Image, Volume 8, Issue 6. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1400.	14.6	7
52	Multireference Approaches for Excited States of Molecules. Chemical Reviews, 2018, 118, 7293-7361.	47.7	287
53	Nonadiabatic dynamics: The SHARC approach. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1370.	14.6	274
54	Intersystem Crossing as a Key Component of the Nonadiabatic Relaxation Dynamics of Bithiophene and Terthiophene. Journal of Chemical Theory and Computation, 2018, 14, 4530-4540.	5.3	17

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55	General Trajectory Surface Hopping Method for Ultrafast Nonadiabatic Dynamics. RSC Theoretical and Computational Chemistry Series, 2018, , 348-385.	0.7	3
56	Ab initio molecular dynamics relaxation and intersystem crossing mechanisms of 5-azacytosine. Physical Chemistry Chemical Physics, 2017, 19, 5888-5894.	2.8	31
57	Ultrafast Electronic Energy Transfer in an Orthogonal Molecular Dyad. Journal of Physical Chemistry Letters, 2017, 8, 1086-1092.	4.6	32
58	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.	4.6	49
59	UV absorption in metal decorated boron nitride flakes: a theoretical analysis of excited states. Molecular Physics, 2017, 115, 2469-2477.	1.7	5
60	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.	5.3	13
61	Solvatochromic Effects on the Absorption Spectrum of 2-Thiocytosine. Journal of Physical Chemistry B, 2017, 121, 5187-5196.	2.6	31
62	2-Thiouracil intersystem crossing photodynamics studied by wavelength-dependent photoelectron and transient absorption spectroscopies. Physical Chemistry Chemical Physics, 2017, 19, 19756-19766.	2.8	58
63	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.	7.4	79
64	Insights into the deactivation of 5-bromouracil after ultraviolet excitation. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2017, 375, 20160202.	3.4	8
65	Evaluation of the quasi correlated tight-binding (QCTB) model for describing polyradical character in polycyclic hydrocarbons. Journal of Chemical Physics, 2017, 146, 064106.	3.0	21
66	Color Fineâ€Tuning of Optical Materials Through Rational Design. ChemPhysChem, 2017, 18, 549-563.	2.1	15
67	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.	2.8	40
68	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.	5.3	40
69	Molecular oxygen observed by direct photoproduction from carbon dioxide. Physical Review A, 2017, 95, .	2.5	13
70	Chromophores from hexeneuronic acids: identification of HexA-derived chromophores. Cellulose, 2017, 24, 3671-3687.	4.9	23
71	Surface hopping dynamics including intersystem crossing using the algebraic diagrammatic construction method. Journal of Chemical Physics, 2017, 147, 184109.	3.0	32
72	Nonadiabatic Dynamics of Cycloparaphenylenes with TD-DFTB Surface Hopping. Journal of Chemical Theory and Computation, 2017, 13, 5846-5860.	5.3	46

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73	Charge-transfer states in triazole linked donorâ€“acceptor materials: strong effects of chemical modification and solvation. Physical Chemistry Chemical Physics, 2017, 19, 18055-18067.	2.8	19
74	The DNA nucleobase thymine in motion â€“ Intersystem crossing simulated with surface hopping. Chemical Physics, 2017, 482, 9-15.	1.9	32
75	Challenges in Simulating Light-Induced Processes in DNA. Molecules, 2017, 22, 49.	3.8	21
76	Entanglement entropy of electronic excitations. Journal of Chemical Physics, 2016, 144, 194107.	3.0	44
77	Communication: Unambiguous comparison of many-electron wavefunctions through their overlaps. Journal of Chemical Physics, 2016, 145, 021103.	3.0	19
78	Photoelectron spectra of 2-thiouracil, 4-thiouracil, and 2,4-dithiouracil. Journal of Chemical Physics, 2016, 144, 074303.	3.0	46
79	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. Journal of Computational Chemistry, 2016, 37, 506-541.	3.3	1,317
80	Internal conversion and intersystem crossing pathways in UV excited, isolated uracils and their implications in prebiotic chemistry. Physical Chemistry Chemical Physics, 2016, 18, 20168-20176.	2.8	65
81	Intersystem Crossing Pathways in the Noncanonical Nucleobase 2-Thiouracil: A Time-Dependent Picture. Journal of Physical Chemistry Letters, 2016, 7, 1978-1983.	4.6	117
82	The origin of efficient triplet state population in sulfur-substituted nucleobases. Nature Communications, 2016, 7, 13077.	12.8	149
83	Revealing Deactivation Pathways Hidden in Time-Resolved Photoelectron Spectra. Scientific Reports, 2016, 6, 35522.	3.3	27
84	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.	2.8	57
85	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.	2.5	91
86	Efficient and Flexible Computation of Many-Electron Wave Function Overlaps. Journal of Chemical Theory and Computation, 2016, 12, 1207-1219.	5.3	145
87	Benzophenone Ultrafast Triplet Population: Revisiting the Kinetic Model by Surface-Hopping Dynamics. Journal of Physical Chemistry Letters, 2016, 7, 622-626.	4.6	89
88	A general method to describe intersystem crossing dynamics in trajectory surface hopping. International Journal of Quantum Chemistry, 2015, 115, 1215-1231.	2.0	228
89	Communication: Exciton analysis in time-dependent density functional theory: How functionals shape excited-state characters. Journal of Chemical Physics, 2015, 143, 171101.	3.0	74
90	Statistical analysis of electronic excitation processes: Spatial location, compactness, charge transfer, and electron-hole correlation. Journal of Computational Chemistry, 2015, 36, 1609-1620.	3.3	95

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91	Intramolecular Charge-Transfer Excited-State Processes in 4-(N,N-Dimethylamino)benzonitrile: The Role of Twisting and the ĭ€Ïƒ* State. Journal of Physical Chemistry A, 2015, 119, 6232-6243.	2.5	60
92	High-Level Ab Initio Computations of the Absorption Spectra of Organic Iridium Complexes. Journal of Physical Chemistry A, 2015, 119, 1023-1036.	2.5	34
93	Electronic and Structural Elements That Regulate the Excited-State Dynamics in Purine Nucleobase Derivatives. Journal of the American Chemical Society, 2015, 137, 4368-4381.	13.7	72
94	A Static Picture of the Relaxation and Intersystem Crossing Mechanisms of Photoexcited 2-Thiouracil. Journal of Physical Chemistry A, 2015, 119, 9524-9533.	2.5	69
95	Ultrafast Intersystem Crossing in SO2 and Nucleobases. Springer Proceedings in Physics, 2015, , 509-513.	0.2	1
96	Excitation of Nucleobases from a Computational Perspective II: Dynamics. Topics in Current Chemistry, 2014, 355, 99-153.	4.0	43
97	Exciton analysis of many-body wave functions: Bridging the gap between the quasiparticle and molecular orbital pictures. Physical Review A, 2014, 90, .	2.5	131
98	Non-adiabatic and intersystem crossing dynamics in SO₂. II. The role of triplet states in the bound state dynamics studied by surface-hopping simulations. Journal of Chemical Physics, 2014, 140, 204302.	3.0	68
99	Perturbational treatment of spin-orbit coupling for generally applicable high-level multi-reference methods. Journal of Chemical Physics, 2014, 141, 074105.	3.0	33
100	Ultrafast intersystem crossing dynamics in uracil unravelled byab initiomolecular dynamics. Physical Chemistry Chemical Physics, 2014, 16, 24423-24436.	2.8	95
101	New tools for the systematic analysis and visualization of electronic excitations. I. Formalism. Journal of Chemical Physics, 2014, 141, 024106.	3.0	369
102	New tools for the systematic analysis and visualization of electronic excitations. II. Applications. Journal of Chemical Physics, 2014, 141, 024107.	3.0	199
103	Surface Hopping Dynamics with Correlated Single-Reference Methods: 9H-Adenine as a Case Study. Journal of Chemical Theory and Computation, 2014, 10, 1395-1405.	5.3	170
104	Newtonâ€<scp>X</scp>: a surfaceâ€hopping program for nonadiabatic molecular dynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 26-33.	14.6	370
105	Ultrafast Intersystem Crossing in SO2 and Nucleobases. , 2014, , .		0
106	Singlet and Triplet Excitedâ€State Dynamics Study of the Keto and Enol Tautomers of Cytosine. ChemPhysChem, 2013, 14, 2920-2931.	2.1	86
107	Electronic excitation and structural relaxation of the adenine dinucleotide in gas phase and solution. Photochemical and Photobiological Sciences, 2013, 12, 1440-1452.	2.9	46
108	The Multiradical Character of Oneâ€and Twoâ€Dimensional Graphene Nanoribbons. Angewandte Chemie - International Edition, 2013, 52, 2581-2584.	13.8	197

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109	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.	3.0	173
110	Analysis of Excitonic and Charge Transfer Interactions from Quantum Chemical Calculations. Journal of Chemical Theory and Computation, 2012, 8, 2777-2789.	5.3	375
111	UV Absorption Spectrum of Alternating DNA Duplexes. Analysis of Excitonic and Charge Transfer Interactions. Journal of Physical Chemistry A, 2012, 116, 11151-11160.	2.5	70
112	Ruthenium(II) Photosensitizers of Tridentate Clickâ€Derived Cyclometalating Ligands: A Joint Experimental and Computational Study. Chemistry - A European Journal, 2012, 18, 4010-4025.	3.3	61
113	Electronically excited states and photodynamics: a continuing challenge. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	77
114	Semiclassical dynamics simulations of charge transport in stacked Ï€-systems. Journal of Chemical Physics, 2011, 134, 034309.	3.0	27
115	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.	2.5	110