

Sebastian Mai

List of Publications by Year in descending order

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115
papers

8,714
citations

57631

44
h-index

43802

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. <i>Molecular Physics</i> , 2023, 121, .	0.8	3
2	libwfa: Wavefunction analysis tools for excited and open-shell electronic states. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2022, 12, .	6.2	16
3	Reversible P=O bond cleavage at an iridium(Ir^{III}) metal centre. <i>Chemical Communications</i> , 2022, 58, 5598-5601.	2.2	3
4	Ultrafast Intersystem Crossing Dynamics of 6-Selenoguanine in Water. <i>Jacs Au</i> , 2022, 2, 1699-1711.	3.6	10
5	Resolving Femtosecond Solvent Reorganization Dynamics in an Iron Complex by Nonadiabatic Dynamics Simulations. <i>Journal of the American Chemical Society</i> , 2022, 144, 12861-12873.	6.6	11
6	Oxygen harvesting from carbon dioxide: simultaneous epoxidation and CO formation. <i>Chemical Science</i> , 2021, 12, 13373-13378.	3.7	5
7	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
8	Excited-State Properties and Relaxation Pathways of Selenium-Substituted Guanine Nucleobase in Aqueous Solution and DNA Duplex. <i>Journal of Physical Chemistry B</i> , 2021, 125, 1778-1789.	1.2	18
9	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
10	A Force Field for a Manganese-Vanadium Water Oxidation Catalyst: Redox Potentials in Solution as Showcase. <i>Catalysts</i> , 2021, 11, 493.	1.6	8
11	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
12	Spectral Signatures of Oxidation States in a Manganese(IV)-Oxo Cubane Water Oxidation Catalyst. <i>Chemistry - A European Journal</i> , 2021, 27, 17078-17086.	1.7	4
13	Surface Hopping Dynamics on Vibronic Coupling Models. <i>Accounts of Chemical Research</i> , 2021, 54, 3760-3771.	7.6	32
14	On the population of triplet states of 2-seleno-thymine. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 5447-5454.	1.3	7
15	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
16	Jahn-Teller Effects in a Vanadate-Stabilized Manganese(IV)-Oxo Cubane Water Oxidation Catalyst. <i>Chemistry - A European Journal</i> , 2021, 27, 17066-17077.	1.7	8
17	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
18	Revealing Ultrafast Population Transfer between Nearly Degenerate Electronic States. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 1443-1449.	2.1	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. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 7483-7488.	2.1	21
20	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
21	Implementation of Coherent Switching with Decay of Mixing into the SHARC Program. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3464-3475.	2.3	18
22	Orbital-free photophysical descriptors to predict directional excitations in metal-based photosensitizers. <i>Chemical Science</i> , 2020, 11, 7685-7693.	3.7	9
23	Competing ultrafast photoinduced electron transfer and intersystem crossing of [Re(CO) ₃ (Dmp)(His124)(Trp122)] ⁺ in <i>Pseudomonas aeruginosa</i> azurin: a nonadiabatic dynamics study. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 65.	0.5	17
24	Multi-Tier 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
25	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
26	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
27	The generality of the GLUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. <i>Journal of Chemical Physics</i> , 2020, 152, 134110.	1.2	42
28	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
29	Molecular Photochemistry: Recent Developments in Theory. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 16832-16846.	7.2	91
30	Molekulare Photochemie: Moderne Entwicklungen in der theoretischen Chemie. <i>Angewandte Chemie</i> , 2020, 132, 16976-16992.	1.6	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. <i>Chemical Science</i> , 2019, 10, 8100-8107.	3.7	140
33	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
34	OpenMolcas: From Source Code to Insight. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5925-5964.	2.3	661
35	Dynamics of benzene excimer formation from the parallel-displaced dimer. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 13916-13924.	1.3	23
36	Highly efficient surface hopping dynamics using a linear vibronic coupling model. <i>Physical Chemistry Chemical Physics</i> , 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. <i>Molecular Systems Design and Engineering</i> , 2019, 4, 951-961.	1.7	13
38	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
39	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
40	Curious Case of 2-Selenouracil: Efficient Population of Triplet States and Yet Photostable. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3730-3742.	2.3	14
41	Visualisation of Electronic Excited-State Correlation in Real Space. <i>ChemPhotoChem</i> , 2019, 3, 702-706.	1.5	16
42	Unconventional two-step spin relaxation dynamics of $[\text{Re}(\text{CO})_3(\text{im})(\text{phen})]^{3+}$ in aqueous solution. <i>Chemical Science</i> , 2019, 10, 10405-10411.	3.7	35
43	Identification of important normal modes in nonadiabatic dynamics simulations by coherence, correlation, and frequency analyses. <i>Journal of Chemical Physics</i> , 2019, 151, 244115.	1.2	16
44	Quantitative wave function analysis for excited states of transition metal complexes. <i>Coordination Chemistry Reviews</i> , 2018, 361, 74-97.	9.5	109
45	Benchmarking Excited-State Calculations Using Exciton Properties. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 710-725.	2.3	128
46	Interstate vibronic coupling constants between electronic excited states for complex molecules. <i>Journal of Chemical Physics</i> , 2018, 148, 124119.	1.2	33
47	Novel Molecular-Dynamics-Based Protocols for Phase Space Sampling in Complex Systems. <i>Frontiers in Chemistry</i> , 2018, 6, 495.	1.8	28
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 within an Exciton Picture. An Electrostatic Embedding Scheme. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 6139-6148.	2.3	29
50	Simulated and Experimental Time-Resolved Photoelectron Spectra of the Intersystem Crossing Dynamics in 2-Thiouracil. <i>Molecules</i> , 2018, 23, 2836.	1.7	28
51	Cover Image, Volume 8, Issue 6. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2018, 8, e1400.	6.2	7
52	Multireference Approaches for Excited States of Molecules. <i>Chemical Reviews</i> , 2018, 118, 7293-7361.	23.0	287
53	Nonadiabatic dynamics: The SHARC approach. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2018, 8, e1370.	6.2	274
54	Intersystem Crossing as a Key Component of the Nonadiabatic Relaxation Dynamics of Bithiophene and Terthiophene. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4530-4540.	2.3	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.	1.3	31
57	Ultrafast Electronic Energy Transfer in an Orthogonal Molecular Dyad. Journal of Physical Chemistry Letters, 2017, 8, 1086-1092.	2.1	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.	2.1	49
59	UV absorption in metal decorated boron nitride flakes: a theoretical analysis of excited states. Molecular Physics, 2017, 115, 2469-2477.	0.8	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.	2.3	13
61	Solvatochromic Effects on the Absorption Spectrum of 2-Thiocytosine. Journal of Physical Chemistry B, 2017, 121, 5187-5196.	1.2	31
62	2-Thiouracil intersystem crossing photodynamics studied by wavelength-dependent photoelectron and transient absorption spectroscopies. Physical Chemistry Chemical Physics, 2017, 19, 19756-19766.	1.3	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.	3.7	79
64	Insights into the deactivation of 5-bromouracil after ultraviolet excitation. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2017, 375, 20160202.	1.6	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.	1.2	21
66	Color Fineâ€“Tuning of Optical Materials Through Rational Design. ChemPhysChem, 2017, 18, 549-563.	1.0	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.	1.3	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.	2.3	40
69	Molecular oxygen observed by direct photoproduction from carbon dioxide. Physical Review A, 2017, 95, .	1.0	13
70	Chromophores from hexeneuronic acids: identification of HexA-derived chromophores. Cellulose, 2017, 24, 3671-3687.	2.4	23
71	Surface hopping dynamics including intersystem crossing using the algebraic diagrammatic construction method. Journal of Chemical Physics, 2017, 147, 184109.	1.2	32
72	Nonadiabatic Dynamics of Cycloparaphenylenes with TD-DFTB Surface Hopping. Journal of Chemical Theory and Computation, 2017, 13, 5846-5860.	2.3	46

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73	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
74	The DNA nucleobase thymine in motion – Intersystem crossing simulated with surface hopping. <i>Chemical Physics</i> , 2017, 482, 9-15.	0.9	32
75	Challenges in Simulating Light-Induced Processes in DNA. <i>Molecules</i> , 2017, 22, 49.	1.7	21
76	Entanglement entropy of electronic excitations. <i>Journal of Chemical Physics</i> , 2016, 144, 194107.	1.2	44
77	Communication: Unambiguous comparison of many-electron wavefunctions through their overlaps. <i>Journal of Chemical Physics</i> , 2016, 145, 021103.	1.2	19
78	Photoelectron spectra of 2-thiouracil, 4-thiouracil, and 2,4-dithiouracil. <i>Journal of Chemical Physics</i> , 2016, 144, 074303.	1.2	46
79	<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
80	Internal conversion and intersystem crossing pathways in UV excited, isolated uracils and their implications in prebiotic chemistry. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 20168-20176.	1.3	65
81	Intersystem Crossing Pathways in the Noncanonical Nucleobase 2-Thiouracil: A Time-Dependent Picture. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1978-1983.	2.1	117
82	The origin of efficient triplet state population in sulfur-substituted nucleobases. <i>Nature Communications</i> , 2016, 7, 13077.	5.8	149
83	Revealing Deactivation Pathways Hidden in Time-Resolved Photoelectron Spectra. <i>Scientific Reports</i> , 2016, 6, 35522.	1.6	27
84	Excitons in poly(para 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
85	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
86	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
87	Benzophenone Ultrafast Triplet Population: Revisiting the Kinetic Model by Surface-Hopping Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 622-626.	2.1	89
88	A general method to describe intersystem crossing dynamics in trajectory surface hopping. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 1215-1231.	1.0	228
89	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
90	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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91	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
92	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
93	Electronic and Structural Elements That Regulate the Excited-State Dynamics in Purine Nucleobase Derivatives. <i>Journal of the American Chemical Society</i> , 2015, 137, 4368-4381.	6.6	72
94	A Static Picture of the Relaxation and Intersystem Crossing Mechanisms of Photoexcited 2-Thiouracil. <i>Journal of Physical Chemistry A</i> , 2015, 119, 9524-9533.	1.1	69
95	Ultrafast Intersystem Crossing in SO ₂ and Nucleobases. <i>Springer Proceedings in Physics</i> , 2015, , 509-513.	0.1	1
96	Excitation of Nucleobases from a Computational Perspective II: Dynamics. <i>Topics in Current Chemistry</i> , 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. <i>Physical Review A</i> , 2014, 90, .	1.0	131
98	Non-adiabatic and intersystem crossing dynamics in SO ₂ . II. The role of triplet states in the bound state dynamics studied by surface-hopping simulations. <i>Journal of Chemical Physics</i> , 2014, 140, 204302.	1.2	68
99	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
100	Ultrafast intersystem crossing dynamics in uracil unravelled by <i>ab initio</i> molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 24423-24436.	1.3	95
101	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
102	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
103	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
104	Newton-X: a surface-hopping program for nonadiabatic molecular dynamics. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2014, 4, 26-33.	6.2	370
105	Ultrafast Intersystem Crossing in SO ₂ and Nucleobases. , 2014, , .		0
106	Singlet and Triplet Excited-State Dynamics Study of the Keto and Enol Tautomers of Cytosine. <i>ChemPhysChem</i> , 2013, 14, 2920-2931.	1.0	86
107	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
108	The Multiradical Character of One- and Two-Dimensional Graphene Nanoribbons. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 2581-2584.	7.2	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. <i>Journal of Chemical Physics</i> , 2012, 137, 22A514.	1.2	173
110	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
111	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
112	Ruthenium(II) Photosensitizers of Tridentate Click-Derived Cyclometalating Ligands: A Joint Experimental and Computational Study. <i>Chemistry - A European Journal</i> , 2012, 18, 4010-4025.	1.7	61
113	Electronically excited states and photodynamics: a continuing challenge. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	77
114	Semiclassical dynamics simulations of charge transport in stacked π -systems. <i>Journal of Chemical Physics</i> , 2011, 134, 034309.	1.2	27
115	Excited-State Diproton Transfer in [2,2'-Bipyridyl]-3,3'-diol: the Mechanism Is Sequential, Not Concerted. <i>Journal of Physical Chemistry A</i> , 2009, 113, 8490-8499.	1.1	110