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	<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
2	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	2.3	661
3	Analysis of Excitonic and Charge Transfer Interactions from Quantum Chemical Calculations. Journal of Chemical Theory and Computation, 2012, 8, 2777-2789.	2.3	375
4	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
5	New tools for the systematic analysis and visualization of electronic excitations. I. Formalism. Journal of Chemical Physics, 2014, 141, 024106.	1.2	369
6	Multireference Approaches for Excited States of Molecules. Chemical Reviews, 2018, 118, 7293-7361.	23.0	287
7	Nonadiabatic dynamics: The SHARC approach. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1370.	6.2	274
8	A general method to describe intersystem crossing dynamics in trajectory surface hopping. International Journal of Quantum Chemistry, 2015, 115, 1215-1231.	1.0	228
9	New tools for the systematic analysis and visualization of electronic excitations. II. Applications. Journal of Chemical Physics, 2014, 141, 024107.	1.2	199
10	The Multiradical Character of Oneâ€•and Twoâ€Dimensional Graphene Nanoribbons. Angewandte Chemie - International Edition, 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. Journal of Chemical Physics, 2012, 137, 22A514.	1.2	173
12	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
13	The origin of efficient triplet state population in sulfur-substituted nucleobases. Nature Communications, 2016, 7, 13077.	5.8	149
14	Efficient and Flexible Computation of Many-Electron Wave Function Overlaps. Journal of Chemical Theory and Computation, 2016, 12, 1207-1219.	2.3	145
15	Machine learning enables long time scale molecular photodynamics simulations. Chemical Science, 2019, 10, 8100-8107.	3.7	140
16	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
17	Benchmarking Excited-State Calculations Using Exciton Properties. Journal of Chemical Theory and Computation, 2018, 14, 710-725.	2.3	128
18	Intersystem Crossing Pathways in the Noncanonical Nucleobase 2-Thiouracil: A Time-Dependent Picture. Journal of Physical Chemistry Letters, 2016, 7, 1978-1983.	2.1	117

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19	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
20	Quantitative wave function analysis for excited states of transition metal complexes. Coordination Chemistry Reviews, 2018, 361, 74-97.	9.5	109
21	Ultrafast intersystem crossing dynamics in uracil unravelled byab initiomolecular dynamics. Physical Chemistry Chemical Physics, 2014, 16, 24423-24436.	1.3	95
22	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
23	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
24	Molecular Photochemistry: Recent Developments in Theory. Angewandte Chemie - International Edition, 2020, 59, 16832-16846.	7.2	91
25	Benzophenone Ultrafast Triplet Population: Revisiting the Kinetic Model by Surface-Hopping Dynamics. Journal of Physical Chemistry Letters, 2016, 7, 622-626.	2.1	89
26	Singlet and Triplet Excitedâ€State Dynamics Study of the Keto and Enol Tautomers of Cytosine. ChemPhysChem, 2013, 14, 2920-2931.	1.0	86
27	Highly efficient surface hopping dynamics using a linear vibronic coupling model. Physical Chemistry Chemical Physics, 2019, 21, 57-69.	1.3	81
28	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
29	Electronically excited states and photodynamics: a continuing challenge. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	77
30	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
31	Electronic and Structural Elements That Regulate the Excited-State Dynamics in Purine Nucleobase Derivatives. Journal of the American Chemical Society, 2015, 137, 4368-4381.	6.6	72
32	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
33	A Static Picture of the Relaxation and Intersystem Crossing Mechanisms of Photoexcited 2-Thiouracil. Journal of Physical Chemistry A, 2015, 119, 9524-9533.	1.1	69
34	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.	1.2	68
35	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.	1.3	65
36	Ruthenium(II) Photosensitizers of Tridentate Clickâ€Derived Cyclometalating Ligands: A Joint Experimental and Computational Study. Chemistry - A European Journal, 2012, 18, 4010-4025.	1.7	61

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37	Intramolecular Charge-Transfer Excited-State Processes in 4-(N,N-Dimethylamino)benzonitrile: The Role of Twisting and the Ï€Ïƒ* State. Journal of Physical Chemistry A, 2015, 119, 6232-6243.	1.1	60
38	Toward an understanding of electronic excitation energies beyond the molecular orbital picture. Physical Chemistry Chemical Physics, 2020, 22, 6058-6080.	1.3	60
39	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
40	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
41	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
42	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
43	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
44	Photoelectron spectra of 2-thiouracil, 4-thiouracil, and 2,4-dithiouracil. Journal of Chemical Physics, 2016, 144, 074303.	1.2	46
45	Nonadiabatic Dynamics of Cycloparaphenylenes with TD-DFTB Surface Hopping. Journal of Chemical Theory and Computation, 2017, 13, 5846-5860.	2.3	46
46	Entanglement entropy of electronic excitations. Journal of Chemical Physics, 2016, 144, 194107.	1.2	44
47	Excitation of Nucleobases from a Computational Perspective II: Dynamics. Topics in Current Chemistry, 2014, 355, 99-153.	4.0	43
48	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	1.2	42
49	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
50	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
51	Unconventional two-step spin relaxation dynamics of [Re(CO)₃(im)(phen)]⁺ in aqueous solution. Chemical Science, 2019, 10, 10405-10411.	3.7	35
52	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
53	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
54	Perturbational treatment of spin-orbit coupling for generally applicable high-level multi-reference methods. Journal of Chemical Physics, 2014, 141, 074105.	1.2	33

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55	Interstate vibronic coupling constants between electronic excited states for complex molecules. Journal of Chemical Physics, 2018, 148, 124119.	1.2	33
56	Ultrafast Electronic Energy Transfer in an Orthogonal Molecular Dyad. Journal of Physical Chemistry Letters, 2017, 8, 1086-1092.	2.1	32
57	Surface hopping dynamics including intersystem crossing using the algebraic diagrammatic construction method. Journal of Chemical Physics, 2017, 147, 184109.	1.2	32
58	The DNA nucleobase thymine in motion â€“ Intersystem crossing simulated with surface hopping. Chemical Physics, 2017, 482, 9-15.	0.9	32
59	Wavelength-optimized Two-Photon Polymerization Using Initiators Based on Multipolar Aminostyryl-1,3,5-triazines. Scientific Reports, 2018, 8, 17273.	1.6	32
60	Surface Hopping Dynamics on Vibronic Coupling Models. Accounts of Chemical Research, 2021, 54, 3760-3771.	7.6	32
61	Ab initio molecular dynamics relaxation and intersystem crossing mechanisms of 5-azacytosine. Physical Chemistry Chemical Physics, 2017, 19, 5888-5894.	1.3	31
62	Solvatochromic Effects on the Absorption Spectrum of 2-Thiocytosine. Journal of Physical Chemistry B, 2017, 121, 5187-5196.	1.2	31
63	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
64	Surface Hopping within an Exciton Picture. An Electrostatic Embedding Scheme. Journal of Chemical Theory and Computation, 2018, 14, 6139-6148.	2.3	29
65	Novel Molecular-Dynamics-Based Protocols for Phase Space Sampling in Complex Systems. Frontiers in Chemistry, 2018, 6, 495.	1.8	28
66	Simulated and Experimental Time-Resolved Photoelectron Spectra of the Intersystem Crossing Dynamics in 2-Thiouracil. Molecules, 2018, 23, 2836.	1.7	28
67	Semiclassical dynamics simulations of charge transport in stacked Ï€-systems. Journal of Chemical Physics, 2011, 134, 034309.	1.2	27
68	Revealing Deactivation Pathways Hidden in Time-Resolved Photoelectron Spectra. Scientific Reports, 2016, 6, 35522.	1.6	27
69	Chromophores from hexeneuronic acids: identification of HexA-derived chromophores. Cellulose, 2017, 24, 3671-3687.	2.4	23
70	Dynamics of benzene excimer formation from the parallel-displaced dimer. Physical Chemistry Chemical Physics, 2019, 21, 13916-13924.	1.3	23
71	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
72	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

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73	Challenges in Simulating Light-Induced Processes in DNA. Molecules, 2017, 22, 49.	1.7	21
74	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.	2.1	21
75	Communication: Unambiguous comparison of many-electron wavefunctions through their overlaps. Journal of Chemical Physics, 2016, 145, 021103.	1.2	19
76	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
77	Implementation of Coherent Switching with Decay of Mixing into the SHARC Program. Journal of Chemical Theory and Computation, 2020, 16, 3464-3475.	2.3	18
78	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.	1.2	18
79	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.	2.3	17
80	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.	0.5	17
81	Visualisation of Electronic Excitedâ€State Correlation in Real Space. ChemPhotoChem, 2019, 3, 702-706.	1.5	16
82	Identification of important normal modes in nonadiabatic dynamics simulations by coherence, correlation, and frequency analyses. Journal of Chemical Physics, 2019, 151, 244115.	1.2	16
83	libwfa: Wavefunction analysis tools for excited and openâ€shell electronic states. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	6.2	16
84	Color Fineâ€Tuning of Optical Materials Through Rational Design. ChemPhysChem, 2017, 18, 549-563.	1.0	15
85	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
86	Curious Case of 2-Selenouracil: Efficient Population of Triplet States and Yet Photostable. Journal of Chemical Theory and Computation, 2019, 15, 3730-3742.	2.3	14
87	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
88	Molecular oxygen observed by direct photoproduction from carbon dioxide. Physical Review A, 2017, 95, .	1.0	13
89	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
90	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

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91	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
92	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
93	Resolving Femtosecond Solvent Reorganization Dynamics in an Iron Complex by Nonadiabatic Dynamics Simulations. Journal of the American Chemical Society, 2022, 144, 12861-12873.	6.6	11
94	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
95	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
96	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
97	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
98	Ultrafast Intersystem Crossing Dynamics of 6-Selenoguanine in Water. Jacs Au, 2022, 2, 1699-1711.	3.6	10
99	Orbital-free photophysical descriptors to predict directional excitations in metal-based photosensitizers. Chemical Science, 2020, 11, 7685-7693.	3.7	9
100	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
101	A Force Field for a Manganese-Vanadium Water Oxidation Catalyst: Redox Potentials in Solution as Showcase. Catalysts, 2021, 11, 493.	1.6	8
102	Jahnâ€Teller Effects in a Vanadateâ€Stabilized Manganeseâ€Oxo Cubane Water Oxidation Catalyst. Chemistry - A European Journal, 2021, 27, 17066-17077.	1.7	8
103	Cover Image, Volume 8, Issue 6. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1400.	6.2	7
104	On the population of triplet states of 2-seleno-thymine. Physical Chemistry Chemical Physics, 2021, 23, 5447-5454.	1.3	7
105	UV absorption in metal decorated boron nitride flakes: a theoretical analysis of excited states. Molecular Physics, 2017, 115, 2469-2477.	0.8	5
106	Revealing Ultrafast Population Transfer between Nearly Degenerate Electronic States. Journal of Physical Chemistry Letters, 2020, 11, 1443-1449.	2.1	5
107	Oxygen harvesting from carbon dioxide: simultaneous epoxidation and CO formation. Chemical Science, 2021, 12, 13373-13378.	3.7	5
108	Spectral Signatures of Oxidation States in a Manganeseâ€Oxo Cubane Water Oxidation Catalyst. Chemistry - A European Journal, 2021, 27, 17078-17086.	1.7	4

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109	General Trajectory Surface Hopping Method for Ultrafast Nonadiabatic Dynamics. RSC Theoretical and Computational Chemistry Series, 2018, , 348-385.	0.7	3
110	Reversible Pâ€“P bond cleavage at an iridium(<scp>iii</scp>) metal centre. Chemical Communications, 2022, 58, 5598-5601.	2.2	3
111	Spin-density calculation via the graphical unitary group approach. Molecular Physics, 2023, 121, .	0.8	3
112	Ultrafast Intersystem Crossing in SO2 and Nucleobases. Springer Proceedings in Physics, 2015, , 509-513.	0.1	1
113	Molekulare Photochemie: Moderne Entwicklungen in der theoretischen Chemie. Angewandte Chemie, 2020, 132, 16976-16992.	1.6	1
114	Ultrafast Intersystem Crossing in SO2 and Nucleobases. , 2014, , .		0
115	Investigation of Complex Relaxation Dynamics of Nearly Degenerated Rydberg States in Acetone. , 2020, , .		0