Andreas Dreuw

List of Publications by Year
in descending order

102 papers	3,047 citations	236925 25 h-index	182427 51 g-index
105 all docs	105 docs citations	105 times ranked	3058 citing authors

#	Article	IF	Citations
1	(Dimesityl)boron Benzodithiophenes: Synthesis, Electrochemical, Photophysical and Theoretical Characterization. ChemistryOpen, 2022, 11, e202100265.	1.9	2
2	Quantum Monte Carlo formulation of the second order algebraic diagrammatic construction: Toward a massively parallel correlated excited state method. Journal of Chemical Physics, 2022, 156, 044105.	3.0	1
3	libwfa: Wavefunction analysis tools for excited and openâ€shell electronic states. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	14.6	16
4	A long-lived fluorenyl cation: efficiency booster for uncaging and photobase properties. Physical Chemistry Chemical Physics, 2022, 24, 5294-5300.	2.8	2
5	Vertical ionization potential benchmark for unitary coupled-cluster and algebraic-diagrammatic construction methods. Journal of Chemical Physics, 2022, 156, 054114.	3.0	8
6	Theoretical analysis and comparison of unitary coupled-cluster and algebraic-diagrammatic construction methods for ionization. Journal of Chemical Physics, 2022, 156, 074104.	3.0	9
7	Exploring the accuracy and usefulness of semi-empirically scaled ADC schemes by blending second and third order terms. Journal of Chemical Physics, 2022, 156, 144101.	3.0	6
8	Stabile Ambipolare Heptacene und deren Redoxâ€Spezies. Angewandte Chemie, 2022, 134, .	2.0	2
9	Persistent Ambipolar Heptacenes and Their Redox Species. Angewandte Chemie - International Edition, 2022, 61, .	13.8	13
10	Accurate Polarization-Resolved Absorption Spectra of Organic Semiconductor Thin Films Using First-Principles Quantum-Chemical Methods: Pentacene as a Case Study. Journal of Physical Chemistry Letters, 2022, 13, 3726-3731.	4.6	11
11	Using core-hole reference states for calculating X-ray photoelectron and emission spectra. Physical Chemistry Chemical Physics, 2022, 24, 11259-11267.	2.8	10
12	Mechanochemically Triggered Topology Changes in Expanded Porphyrins. Chemistry - A European Journal, 2021, 27, 3397-3406.	3.3	14
13	Modeling Molecules under Pressure with Gaussian Potentials. Journal of Chemical Theory and Computation, 2021, 17, 583-597.	5.3	17
14	Experimental and theoretical studies on gold(<scp>iii</scp>) carbonyl complexes: reductive C,H- and C,C bond formation. Dalton Transactions, 2021, 50, 8752-8760.	3.3	6
15	Electronic circular dichroism spectra using the algebraic diagrammatic construction schemes of the polarization propagator up to third order. Journal of Chemical Physics, 2021, 154, 064107.	3.0	12
16	XABOOM: An X-ray Absorption Benchmark of Organic Molecules Based on Carbon, Nitrogen, and Oxygen 1s â†' Ï€* Transitions. Journal of Chemical Theory and Computation, 2021, 17, 1618-1637.	5.3	37
17	Deciphering excited state properties utilizing algebraic diagrammatic construction schemes of decreasing order. Journal of Computational Chemistry, 2021, 42, 793-800.	3.3	3
18	Influence of Core Halogenation on the Electronic Structure of Naphthothiadiazole Derivatives. Journal of Physical Chemistry C, 2021, 125, 6359-6366.	3.1	5

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19	Intermediate state representation approach to physical properties of molecular electron-attached states: Theory, implementation, and benchmarking. Journal of Chemical Physics, 2021, 154, 104117.	3.0	15
20	Gator: A Pythonâ€driven program for spectroscopy simulations using correlated wave functions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1528.	14.6	16
21	Unitary coupled-cluster approach for the calculation of core-excited states and x-ray absorption spectra. Journal of Chemical Physics, 2021, 154, 154108.	3.0	4
22	Embelinâ€™s Versatile Photochemistry Makes It a Potent Photosensitizer for Photodynamic Therapy. Journal of Physical Chemistry B, 2021, 125, 3527-3537.	2.6	2
23	Ab Initio Excited-State Electronic Circular Dichroism Spectra Exploiting the Third-Order Algebraic-Diagrammatic Construction Scheme for the Polarization Propagator. Journal of Physical Chemistry Letters, 2021, 12, 5132-5137.	4.6	8
24	Efficient Open-Source Implementations of Linear-Scaling Polarizable Embedding: Use Octrees to Save the Trees. Journal of Chemical Theory and Computation, 2021, 17, 3445-3454.	5.3	7
25	Designing Force Probes Based on Reversible 6Ï€-Electrocyclizations in Polyenes Using Quantum Chemical Calculations. Journal of Organic Chemistry, 2021, 86, 7477-7489.	3.2	5
26	Geometry dependence of excitonic couplings and the consequences for configurationâ€space sampling. Journal of Computational Chemistry, 2021, 42, 1402-1418.	3.3	5
27	Benchmark of the Extension of Frozen-Density Embedding Theory to Nonvariational Correlated Methods: The Embedded-MP2 Case. Journal of Chemical Theory and Computation, 2021, 17, 4049-4062.	5.3	4
28	Analytical gradients for core-excited states in the algebraic diagrammatic construction (ADC) framework. Journal of Chemical Physics, 2021, 155, 044106.	3.0	4
29	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
30	CAP/EA-ADC method for metastable anions: Computational aspects and application to Ï€* resonances of norbornadiene and 1,4-cyclohexadiene. Journal of Chemical Physics, 2021, 155, 054103.	3.0	13
31	Tailoring the Properties of Optical Force Probes for Polymer Mechanochemistry. Chemistry - A European Journal, 2021, 27, 15889-15897.	3.3	35
32	Rethinking Uncaging: A New Antiaromatic Photocage Driven by a Gain of Resonance Energy. Chemistry - A European Journal, 2021, 27, 14121-14127.	3.3	7
33	Tailoring the Properties of Optical Force Probes for Polymer Mechanochemistry. Chemistry - A European Journal, 2021, 27, 15827-15828.	3.3	12
34	Structure Set in Stone: Designing Rigid Linkers to Control the Efficiency of Intramolecular Singlet Fission. Journal of Physical Chemistry B, 2021, 125, 13235-13245.	2.6	5
35	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCE<scp>ngine</scp>): Automation and interoperability among computational chemistry programs. Journal of Chemical Physics, 2021, 155, 204801.	3.0	15
36	Frontispiece: Tailoring the Properties of Optical Force Probes for Polymer Mechanochemistry. Chemistry - A European Journal, 2021, 27, .	3.3	1

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37	Thiophenylazobenzene: An Alternative Photoisomerization Controlled by Loneâ€Pairâ‹…â‹…â‹…Ï€ Interaction. Angewandte Chemie - International Edition, 2020, 59, 380-387.	13.8	35
38	Thiophenylazobenzene: An Alternative Photoisomerization Controlled by Loneâ€Pairâ‹…â‹…â‹…Ï€ Interaction. Angewandte Chemie, 2020, 132, 388-395.	2.0	9
39	Evaluation of Single-Reference DFT-Based Approaches for the Calculation of Spectroscopic Signatures of Excited States Involved in Singlet Fission. Journal of Physical Chemistry A, 2020, 124, 8446-8460.	2.5	10
40	Interatomic and Intermolecular Coulombic Decay. Chemical Reviews, 2020, 120, 11295-11369.	47.7	106
41	A Doubly Bridged Bis(phenylethynyl)benzene: Different from a Twisted Tolan. Chemistry - A European Journal, 2020, 26, 16990-16993.	3.3	4
42	Complex excited state polarizabilities in the ADC/ISR framework. Journal of Chemical Physics, 2020, 153, 074112.	3.0	9
43	Homoconjugation and Intramolecular Charge Transfer in Extended Aromatic Triptycenes with Different Ï€-Planes. Journal of Organic Chemistry, 2020, 85, 15256-15272.	3.2	24
44	Unitary coupled cluster ground- and excited-state molecular properties. Journal of Chemical Physics, 2020, 153, 084112.	3.0	17
45	Third-Order Unitary Coupled Cluster (UCC3) for Excited Electronic States: Efficient Implementation and Benchmarking. Journal of Chemical Theory and Computation, 2020, 16, 3654-3663.	5.3	11
46	Electronic Properties of 6,13-Diazapentacene Adsorbed on Au(111): A Quantitative Determination of Transport, Singlet and Triplet States, and Electronic Spectra. Journal of Physical Chemistry C, 2020, 124, 13196-13205.	3.1	11
47	The rupture mechanism of rubredoxin is more complex than previously thought. Chemical Science, 2020, 11, 6036-6044.	7.4	1
48	Quinoidal Azaacenes: 99â€‰% Diradical Character. Angewandte Chemie - International Edition, 2020, 59, 12396-12401.	13.8	30
49	Hermitian second-order methods for excited electronic states: Unitary coupled cluster in comparison with algebraicâ€“diagrammatic construction schemes. Journal of Chemical Physics, 2020, 152, 094106.	3.0	12
50	Intermediate state representation approach to physical properties of molecular electron-detached states. I. Theory and implementation. Journal of Chemical Physics, 2020, 152, 024113.	3.0	23
51	RÃ¼cktitelbild: Quinoidal Azaacenes: 99â€‰% Diradical Character (Angew. Chem. 30/2020). Angewandte Chemie, 2020, 132, 12644-12644.	2.0	0
52	Intermediate state representation approach to physical properties of molecular electron-detached states. II. Benchmarking. Journal of Chemical Physics, 2020, 152, 024125.	3.0	15
53	AFM-IR and IR-SNOM for the Characterization of Small Molecule Organic Semiconductors. Journal of Physical Chemistry C, 2020, 124, 5331-5344.	3.1	29
54	Quinoidal Azaacenes: 99â€‰% Diradical Character. Angewandte Chemie, 2020, 132, 12496-12501.	2.0	10

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55	Twisting and bending photo-excited phenylethynylbenzenes â€“ a theoretical analysis. Physical Chemistry Chemical Physics, 2020, 22, 9974-9981.	2.8	6
56	Probing competing relaxation pathways in malonaldehyde with transient X-ray absorption spectroscopy. Chemical Science, 2020, 11, 4180-4193.	7.4	29
57	Ultrafast Singlet Fission in Rigid Azaarene Dimers with Negligible Orbital Overlap. Journal of Physical Chemistry B, 2020, 124, 9163-9174.	2.6	12
58	Analytic nuclear gradients of the algebraic-diagrammatic construction scheme for the polarization propagator up to third order of perturbation theory. Journal of Chemical Physics, 2019, 150, 174110.	3.0	8
59	Similarities and differences of the Lagrange formalism and the intermediate state representation in the treatment of molecular properties. Journal of Chemical Physics, 2019, 150, 164125.	3.0	15
60	CPPE: An Open-Source C++ and Python Library for Polarizable Embedding. Journal of Chemical Theory and Computation, 2019, 15, 6154-6163.	5.3	20
61	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
62	Excited state dynamics of the s-trans-1, 3-butadiene cation: An ab initio quantum dynamical analysis. Journal of Chemical Physics, 2019, 151, 104105.	3.0	0
63	Electronâ€“Hole Correlation as Unambiguous and Universal Classification for the Nature of Low-Lying Ï€Ï€* States of Nitrogen Heterocycles. Journal of Physical Chemistry Letters, 2019, 10, 6112-6117.	4.6	15
64	Density-based descriptors and exciton analyses for visualizing and understanding the electronic structure of excited states. Physical Chemistry Chemical Physics, 2019, 21, 2843-2856.	2.8	34
65	Algebraic diagrammatic construction for the polarisation propagator in combination with effective fragment potentials. Physical Chemistry Chemical Physics, 2019, 21, 3683-3694.	2.8	5
66	Optical Spectra and Fluorescence Quenching in Azaacenes Bearing Fiveâ€Membered Rings. ChemPhotoChem, 2019, 3, 755-762.	3.0	6
67	Tailoring Ultrafast Singlet Fission by the Chemical Modification of Phenazinothiadiazoles. Journal of the American Chemical Society, 2019, 141, 8834-8845.	13.7	39
68	Algebraic-diagrammatic construction scheme for the polarization propagator including ground-state coupled-cluster amplitudes. II. Static polarizabilities. Journal of Chemical Physics, 2019, 150, 174105.	3.0	13
69	Algebraic-diagrammatic construction scheme for the polarization propagator including ground-state coupled-cluster amplitudes. I. Excitation energies. Journal of Chemical Physics, 2019, 150, 174104.	3.0	11
70	Isomerization Dynamics of Electronically Coupled but Thermodynamically Decoupled Bisazobenzenes. ChemPhotoChem, 2019, 3, 411-417.	3.0	6
71	Extension of frozen-density embedding theory for non-variational embedded wavefunctions. Journal of Chemical Physics, 2019, 150, 121101.	3.0	9
72	Efficient implementation of the non-Dyson third-order algebraic diagrammatic construction approximation for the electron propagator for closed- and open-shell molecules. Journal of Chemical Physics, 2019, 150, 064108.	3.0	29

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73	Singlet Fission in Tetraaza-TIPS-Pentacene Oligomers: From fs Excitation to Î¼s Triplet Decay via the Biexcitonic State. Journal of Physical Chemistry B, 2019, 123, 10780-10793.	2.6	24
74	Lewis Acid Catalyzed Enantioselective Photochemical Rearrangements on the Singlet Potential Energy Surface. Journal of the American Chemical Society, 2019, 141, 20053-20057.	13.7	34
75	Simulating X-ray Emission Spectroscopy with Algebraic Diagrammatic Construction Schemes for the Polarization Propagator. Journal of Chemical Theory and Computation, 2019, 15, 546-556.	5.3	29
76	[6Ï€] Photocyclization to cis-Hexahydrocarbazol-4-ones: Substrate Modification, Mechanism, and Scope. Journal of Organic Chemistry, 2019, 84, 1139-1153.	3.2	23
77	A red-shifted two-photon-only caging group for three-dimensional photorelease. Chemical Science, 2018, 9, 2797-2802.	7.4	32
78	Characterizing Bonding Patterns in Diradicals and Triradicals by Density-Based Wave Function Analysis: A Uniform Approach. Journal of Chemical Theory and Computation, 2018, 14, 638-648.	5.3	35
79	Mechanism and cis/trans Selectivity of Vinylogous Nazarov-type [6Ï€] Photocyclizations. Journal of Organic Chemistry, 2018, 83, 964-972.	3.2	16
80	Benchmarking Excited-State Calculations Using Exciton Properties. Journal of Chemical Theory and Computation, 2018, 14, 710-725.	5.3	128
81	Computational design of a molecular triple photoswitch for wavelength-selective control. Chemical Science, 2018, 9, 8665-8672.	7.4	29
82	Substituting Coumarins for Quinolinones: Altering the Cycloreversion Potential Energy Landscape. Journal of Physical Chemistry A, 2018, 122, 7587-7597.	2.5	8
83	Toward quantum-chemical method development for arbitrary basis functions. Journal of Chemical Physics, 2018, 149, 084106.	3.0	10
84	The All-Seeing Eye of Resonant Auger Electron Spectroscopy: A Study on Aqueous Solution Using Tender X-rays. Journal of Physical Chemistry Letters, 2018, 9, 4457-4462.	4.6	6
85	Twist and Returnâ^'Induced Ring Strain Triggers Quick Relaxation of a (Z)-Stabilized Cyclobisazobenzene. Journal of Physical Chemistry Letters, 2018, 9, 4776-4781.	4.6	17
86	Polarizable Embedding Combined with the Algebraic Diagrammatic Construction: Tackling Excited States in Biomolecular Systems. Journal of Chemical Theory and Computation, 2018, 14, 4870-4883.	5.3	26
87	Meltdown! Local Heating by Decaying Excited Host Positive Polarons Triggers Aggregation Quenching in Blue PhOLEDs. ChemPhysChem, 2018, 19, 2961-2966.	2.1	6
88	Benchmark of Excitation Energy Shifts from Frozen-Density Embedding Theory: Introduction of a Density-Overlap-Based Applicability Threshold. Journal of Chemical Theory and Computation, 2018, 14, 4028-4040.	5.3	16
89	Simulating X-ray Spectroscopies and Calculating Core-Excited States of Molecules. Chemical Reviews, 2018, 118, 7208-7248.	47.7	214
90	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

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91	Regular and red-shifted fluorescence of the donorâ€“acceptor compound 5-(1H-pyrrole-1-yl)thiophenecarbonitrile (TCN) is efficiently quenched by internal modes of thiophene. Physical Chemistry Chemical Physics, 2017, 19, 13951-13959.	2.8	3
92	A theoretical study on the mechanistic highlights behind the BrÃ¸nsted-acid dependent merâ€“fac isomerization of homoleptic carbenic iridium complexes for PhOLEDs. Dalton Transactions, 2017, 46, 7194-7209.	3.3	5
93	Force-induced retro-click reaction of triazoles competes with adjacent single-bond rupture. Chemical Science, 2017, 8, 5567-5575.	7.4	20
94	Quantum Chemical Strain Analysis For Mechanochemical Processes. Accounts of Chemical Research, 2017, 50, 1041-1048.	15.6	35
95	Evaluation of the restricted virtual space approximation in the algebraicâ€diagrammatic construction scheme for the polarization propagator to speedâ€up excitedâ€state calculations. Journal of Computational Chemistry, 2017, 38, 1528-1537.	3.3	10
96	Molecular Mechanism of Flavin Photoprotection by Archaeal Dodecin: Photoinduced Electron Transfer and Mg²⁺-Promoted Proton Transfer. Journal of Physical Chemistry B, 2017, 121, 10457-10466.	2.6	7
97	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
98	Resonant Inelastic X-ray Scattering Amplitudes and Cross Sections in the Algebraic Diagrammatic Construction/Intermediate State Representation (ADC/ISR) Approach. Journal of Chemical Theory and Computation, 2017, 13, 5552-5559.	5.3	40
99	Spin the light off: rapid internal conversion into a dark doublet state quenches the fluorescence of an RNA spin label. Physical Chemistry Chemical Physics, 2017, 19, 26255-26264.	2.8	8
100	Implementation and Application of the Frozen Density Embedding Theory with the Algebraic Diagrammatic Construction Scheme for the Polarization Propagator up to Third Order. Journal of Chemical Theory and Computation, 2017, 13, 4711-4725.	5.3	21
101	Regular Fluorescence of 4-Fluoro-N,N-dimethylaniline: No Charge Transfer and No Twisting. Journal of Physical Chemistry A, 2017, 121, 5834-5841.	2.5	4
102	The Spin-Flip Variant of the Algebraic-Diagrammatic Construction Yields the Correct Topology of S₁/S₀ Conical Intersections. Journal of Chemical Theory and Computation, 2017, 13, 4436-4441.	5.3	28