Andreas Dreuw

List of Publications by Year in Descending Order

96 papers	1,483 citations	17 h-index	35 g-index
105 ext. papers	2,178 ext. citations	6.6 avg, IF	5.41 L-index

#	Paper	IF	Citations
96	(Dimesityl)boron Benzodithiophenes: Synthesis, Electrochemical, Photophysical and Theoretical Characterization.. *ChemistryOpen*, **2022**, 11, e202100265	2.3	0
95	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	3.9	1
94	Vertical ionization potential benchmark for unitary coupled-cluster and algebraic-diagrammatic construction methods.. *Journal of Chemical Physics*, **2022**, 156, 054114	3.9	2
93	Theoretical analysis and comparison of unitary coupled-cluster and algebraic-diagrammatic construction methods for ionization.. *Journal of Chemical Physics*, **2022**, 156, 074104	3.9	1
92	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	3.9	1
91	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**, 3726-3731	6.4	1
90	Tailoring the Properties of Optical Force Probes for Polymer Mechanochemistry. *Chemistry - A European Journal*, **2021**, 27, 15827-15828	4.8	0
89	Structure Set in Stone: Designing Rigid Linkers to Control the Efficiency of Intramolecular Singlet Fission. *Journal of Physical Chemistry B*, **2021**, 125, 13235-13245	3.4	0
88	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCEngine): Automation and interoperability among computational chemistry programs. *Journal of Chemical Physics*, **2021**, 155, 204801	3.9	3
87	Influence of Core Halogenation on the Electronic Structure of Naphthothiadiazole Derivatives. *Journal of Physical Chemistry C*, **2021**, 125, 6359-6366	3.8	1
86	Intermediate state representation approach to physical properties of molecular electron-attached states: Theory, implementation, and benchmarking. *Journal of Chemical Physics*, **2021**, 154, 104117	3.9	5
85	Gator: A Python-driven program for spectroscopy simulations using correlated wave functions. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1528	7.9	4
84	Unitary coupled-cluster approach for the calculation of core-excited states and x-ray absorption spectra. *Journal of Chemical Physics*, **2021**, 154, 154108	3.9	1
83	Embelin Versatile Photochemistry Makes It a Potent Photosensitizer for Photodynamic Therapy. *Journal of Physical Chemistry B*, **2021**, 125, 3527-3537	3.4	1
82	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	6.4	1
81	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	6.4	2
80	Designing Force Probes Based on Reversible 6Electrocyclizations in Polyenes Using Quantum Chemical Calculations. *Journal of Organic Chemistry*, **2021**, 86, 7477-7489	4.2	3

79	Geometry dependence of excitonic couplings and the consequences for configuration-space sampling. *Journal of Computational Chemistry*, **2021**, 42, 1402-1418	3.5	1
78	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	6.4	0
77	Analytical gradients for core-excited states in the algebraic diagrammatic construction (ADC) framework. *Journal of Chemical Physics*, **2021**, 155, 044106	3.9	0
76	Mechanochemically Triggered Topology Changes in Expanded Porphyrins. *Chemistry - A European Journal*, **2021**, 27, 3397-3406	4.8	8
75	Modeling Molecules under Pressure with Gaussian Potentials. *Journal of Chemical Theory and Computation*, **2021**, 17, 583-597	6.4	5
74	Experimental and theoretical studies on gold(III) carbonyl complexes: reductive C,H- and C,C bond formation. *Dalton Transactions*, **2021**, 50, 8752-8760	4.3	2
73	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	3.9	4
72	XABOOM: An X-ray Absorption Benchmark of Organic Molecules Based on Carbon, Nitrogen, and Oxygen 1s -π* Transitions. *Journal of Chemical Theory and Computation*, **2021**, 17, 1618-1637	6.4	13
71	Deciphering excited state properties utilizing algebraic diagrammatic construction schemes of decreasing order. *Journal of Computational Chemistry*, **2021**, 42, 793-800	3.5	0
70	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801	3.9	115
69	CAP/EA-ADC method for metastable anions: Computational aspects and application to π* resonances of norbornadiene and 1,4-cyclohexadiene. *Journal of Chemical Physics*, **2021**, 155, 054103	3.9	2
68	Tailoring the Properties of Optical Force Probes for Polymer Mechanochemistry. *Chemistry - A European Journal*, **2021**, 27, 15889-15897	4.8	15
67	Rethinking Uncaging: A New Antiaromatic Photocage Driven by a Gain of Resonance Energy. *Chemistry - A European Journal*, **2021**, 27, 14121-14127	4.8	1
66	Homoconjugation and Intramolecular Charge Transfer in Extended Aromatic Triptycenes with Different π-Planes. *Journal of Organic Chemistry*, **2020**, 85, 15256-15272	4.2	13
65	Unitary coupled cluster ground- and excited-state molecular properties. *Journal of Chemical Physics* , **2020**, 153, 084112	3.9	8
64	Third-Order Unitary Coupled Cluster (UCC3) for Excited Electronic States: Efficient Implementation and Benchmarking. *Journal of Chemical Theory and Computation*, **2020**, 16, 3654-3663	6.4	6
63	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	3.8	5
62	The rupture mechanism of rubredoxin is more complex than previously thought. *Chemical Science*, **2020**, 11, 6036-6044	9.4	0

61	Quinoidal Azaacenes: 99 % Diradical Character. *Angewandte Chemie - International Edition*, **2020**, 59, 12396-12401	16.1	107
60	Hermitian second-order methods for excited electronic states: Unitary coupled cluster in comparison with algebraic-diagrammatic construction schemes. *Journal of Chemical Physics*, **2020**, 152, 094106	3.9	8
59	Intermediate state representation approach to physical properties of molecular electron-detached states. I. Theory and implementation. *Journal of Chemical Physics*, **2020**, 152, 024113	3.9	15
58	R□ktitelbild: Quinoidal Azaacenes: 99 % Diradical Character (Angew. Chem. 30/2020). *Angewandte Chemie*, **2020**, 132, 12644-12644	3.6	
57	Intermediate state representation approach to physical properties of molecular electron-detached states. II. Benchmarking. *Journal of Chemical Physics*, **2020**, 152, 024125	3.9	9
56	AFM-IR and IR-SNOM for the Characterization of Small Molecule Organic Semiconductors. *Journal of Physical Chemistry C*, **2020**, 124, 5331-5344	3.8	16
55	Quinoidal Azaacenes: 99 % Diradical Character. *Angewandte Chemie*, **2020**, 132, 12496-12501	3.6	4
54	Twisting and bending photo-excited phenylethynylbenzenes - a theoretical analysis. *Physical Chemistry Chemical Physics*, **2020**, 22, 9974-9981	3.6	2
53	Ultrafast Singlet Fission in Rigid Azaarene Dimers with Negligible Orbital Overlap. *Journal of Physical Chemistry B*, **2020**, 124, 9163-9174	3.4	5
52	Thiophenylazobenzene: An Alternative Photoisomerization Controlled by Lone-Pair???□Interaction. *Angewandte Chemie*, **2020**, 132, 388-395	3.6	7
51	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	2.8	6
50	Interatomic and Intermolecular Coulombic Decay. *Chemical Reviews*, **2020**, 120, 11295-11369	68.1	31
49	A Doubly Bridged Bis(phenylethynyl)benzene: Different from a Twisted Tolan. *Chemistry - A European Journal*, **2020**, 26, 16990-16993	4.8	1
48	Complex excited state polarizabilities in the ADC/ISR framework. *Journal of Chemical Physics*, **2020**, 153, 074112	3.9	4
47	Thiophenylazobenzene: An Alternative Photoisomerization Controlled by Lone-Pair???□Interaction. *Angewandte Chemie - International Edition*, **2020**, 59, 380-387	16.4	16
46	Probing competing relaxation pathways in malonaldehyde with transient X-ray absorption spectroscopy. *Chemical Science*, **2020**, 11, 4180-4193	9.4	11
45	OpenMolcas: From Source Code to Insight. *Journal of Chemical Theory and Computation*, **2019**, 15, 5925-5964	5.4	310
44	Excited state dynamics of the s-trans-1, 3-butadiene cation: An ab initio quantum dynamical analysis. *Journal of Chemical Physics*, **2019**, 151, 104105	3.9	

43	Electron-Hole Correlation as Unambiguous and Universal Classification for the Nature of Low-Lying π States of Nitrogen Heterocycles. *Journal of Physical Chemistry Letters*, **2019**, 10, 6112-6117	6.4	10
42	Density-based descriptors and exciton analyses for visualizing and understanding the electronic structure of excited states. *Physical Chemistry Chemical Physics*, **2019**, 21, 2843-2856	3.6	23
41	Algebraic diagrammatic construction for the polarisation propagator in combination with effective fragment potentials. *Physical Chemistry Chemical Physics*, **2019**, 21, 3683-3694	3.6	3
40	Optical Spectra and Fluorescence Quenching in Azaacenes Bearing Five-Membered Rings. *ChemPhotoChem*, **2019**, 3, 755-762	3.3	5
39	Tailoring Ultrafast Singlet Fission by the Chemical Modification of Phenazinothiadiazoles. *Journal of the American Chemical Society*, **2019**, 141, 8834-8845	16.4	26
38	Algebraic-diagrammatic construction scheme for the polarization propagator including ground-state coupled-cluster amplitudes. II. Static polarizabilities. *Journal of Chemical Physics*, **2019**, 150, 174105	3.9	11
37	Algebraic-diagrammatic construction scheme for the polarization propagator including ground-state coupled-cluster amplitudes. I. Excitation energies. *Journal of Chemical Physics*, **2019**, 150, 174104	3.9	11
36	Isomerization Dynamics of Electronically Coupled but Thermodynamically Decoupled Bisazobenzenes. *ChemPhotoChem*, **2019**, 3, 411-417	3.3	1
35	Extension of frozen-density embedding theory for non-variational embedded wavefunctions. *Journal of Chemical Physics*, **2019**, 150, 121101	3.9	6
34	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	3.9	17
33	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	3.9	6
32	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	3.9	9
31	CPPE: An Open-Source C++ and Python Library for Polarizable Embedding. *Journal of Chemical Theory and Computation*, **2019**, 15, 6154-6163	6.4	13
30	Singlet Fission in Tetraaza-TIPS-Pentacene Oligomers: From fs Excitation to ns Triplet Decay via the Biexcitonic State. *Journal of Physical Chemistry B*, **2019**, 123, 10780-10793	3.4	13
29	Lewis Acid Catalyzed Enantioselective Photochemical Rearrangements on the Singlet Potential Energy Surface. *Journal of the American Chemical Society*, **2019**, 141, 20053-20057	16.4	19
28	Simulating X-ray Emission Spectroscopy with Algebraic Diagrammatic Construction Schemes for the Polarization Propagator. *Journal of Chemical Theory and Computation*, **2019**, 15, 546-556	6.4	16
27	[6]Photocyclization to cis-Hexahydrocarbazol-4-ones: Substrate Modification, Mechanism, and Scope. *Journal of Organic Chemistry*, **2019**, 84, 1139-1153	4.2	10
26	A red-shifted two-photon-only caging group for three-dimensional photorelease. *Chemical Science*, **2018**, 9, 2797-2802	9.4	25

25	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	6.4	29
24	Mechanism and cis/trans Selectivity of Vinylogous Nazarov-type [6]Photocyclizations *Journal of Organic Chemistry*, **2018**, 83, 964-972	4.2	13
23	Benchmarking Excited-State Calculations Using Exciton Properties. *Journal of Chemical Theory and Computation*, **2018**, 14, 710-725	6.4	97
22	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	6.4	5
21	Twist and Return-Induced Ring Strain Triggers Quick Relaxation of a (Z)-Stabilized Cyclobisazobenzene. *Journal of Physical Chemistry Letters*, **2018**, 9, 4776-4781	6.4	13
20	Polarizable Embedding Combined with the Algebraic Diagrammatic Construction: Tackling Excited States in Biomolecular Systems. *Journal of Chemical Theory and Computation*, **2018**, 14, 4870-4883	6.4	18
19	Meltdown! Local Heating by Decaying Excited Host Positive Polarons Triggers Aggregation Quenching in Blue PhOLEDs. *ChemPhysChem*, **2018**, 19, 2961-2966	3.2	6
18	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	6.4	11
17	Simulating X-ray Spectroscopies and Calculating Core-Excited States of Molecules. *Chemical Reviews*, **2018**, 118, 7208-7248	68.1	140
16	Computational design of a molecular triple photoswitch for wavelength-selective control. *Chemical Science*, **2018**, 9, 8665-8672	9.4	18
15	Substituting Coumarins for Quinolinones: Altering the Cycloreversion Potential Energy Landscape. *Journal of Physical Chemistry A*, **2018**, 122, 7587-7597	2.8	8
14	Toward quantum-chemical method development for arbitrary basis functions. *Journal of Chemical Physics*, **2018**, 149, 084106	3.9	6
13	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	6.4	34
12	Regular and red-shifted fluorescence of the donor-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	3.6	2
11	A theoretical study on the mechanistic highlights behind the Brønsted-acid dependent mer-fac isomerization of homoleptic carbenic iridium complexes for PhOLEDs. *Dalton Transactions*, **2017**, 46, 7194-7209	4.3	4
10	Force-induced retro-click reaction of triazoles competes with adjacent single-bond rupture. *Chemical Science*, **2017**, 8, 5567-5575	9.4	16
9	Quantum Chemical Strain Analysis For Mechanochemical Processes. *Accounts of Chemical Research*, **2017**, 50, 1041-1048	24.3	27
8	Evaluation of the restricted virtual space approximation in the algebraic-diagrammatic construction scheme for the polarization propagator to speed-up excited-state calculations. *Journal of Computational Chemistry*, **2017**, 38, 1528-1537	3.5	9

7	Molecular Mechanism of Flavin Photoprotection by Archaeal Dodecin: Photoinduced Electron Transfer and Mg-Promoted Proton Transfer. *Journal of Physical Chemistry B*, **2017**, 121, 10457-10466	3.4	5
6	Detailed Wave Function Analysis for Multireference Methods: Implementation in the Molcas Program Package and Applications to Tetracene. *Journal of Chemical Theory and Computation*, **2017**, 13, 5343-5353	6.4	32
5	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	6.4	27
4	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	3.6	6
3	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	6.4	14
2	Regular Fluorescence of 4-Fluoro-N,N-dimethylaniline: No Charge Transfer and No Twisting. *Journal of Physical Chemistry A*, **2017**, 121, 5834-5841	2.8	3
1	The Spin-Flip Variant of the Algebraic-Diagrammatic Construction Yields the Correct Topology of S/S Conical Intersections. *Journal of Chemical Theory and Computation*, **2017**, 13, 4436-4441	6.4	22