Christoph Bannwarth

List of Publications by Year
in descending order

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54	9,031	159585	155660
papers	citations	30 h-index	55 g-index

67	67	67	7563
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	GFN2-xTBâ€"An Accurate and Broadly Parametrized Self-Consistent Tight-Binding Quantum Chemical Method with Multipole Electrostatics and Density-Dependent Dispersion Contributions. Journal of Chemical Theory and Computation, 2019, 15, 1652-1671.	5.3	1,704
2	A Robust and Accurate Tight-Binding Quantum Chemical Method for Structures, Vibrational Frequencies, and Noncovalent Interactions of Large Molecular Systems Parametrized for All spd-Block Elements (Z = 1â€"86). Journal of Chemical Theory and Computation, 2017, 13, 1989-2009.	5.3	1,072
3	Dispersion-Corrected Mean-Field Electronic Structure Methods. Chemical Reviews, 2016, 116, 5105-5154.	47.7	1,032
4	A generally applicable atomic-charge dependent London dispersion correction. Journal of Chemical Physics, 2019, 150, 154122.	3.0	697
5	Extension of the D3 dispersion coefficient model. Journal of Chemical Physics, 2017, 147, 034112.	3.0	617
6	Consistent structures and interactions by density functional theory with small atomic orbital basis sets. Journal of Chemical Physics, 2015, 143, 054107.	3.0	605
7	Extended <scp>tightâ€binding</scp> quantum chemistry methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1493.	14.6	596
8	B97-3c: A revised low-cost variant of the B97-D density functional method. Journal of Chemical Physics, 2018, 148, 064104.	3.0	400
9	A simplified time-dependent density functional theory approach for electronic ultraviolet and circular dichroism spectra of very large molecules. Computational and Theoretical Chemistry, 2014, 1040-1041, 45-53.	2.5	211
10	Combinations of Ethers and B(C₆F₅)₃ Function as Hydrogenation Catalysts. Angewandte Chemie - International Edition, 2013, 52, 7492-7495.	13.8	180
11	Catalytic deracemization of chiral allenes by sensitized excitation with visible light. Nature, 2018, 564, 240-243.	27.8	180
12	Fully Automated Quantumâ€Chemistryâ€Based Computation of Spinâ€"Spinâ€Coupled Nuclear Magnetic Resonance Spectra. Angewandte Chemie - International Edition, 2017, 56, 14763-14769.	13.8	158
13	<scp>TeraChem</scp>: A graphical processing unit<scp>â€accelerated</scp> electronic structure package for <scp>largeâ€scale</scp> ab initio molecular dynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1494.	14.6	143
14	Ultra-fast computation of electronic spectra for large systems by tight-binding based simplified Tamm-Dancoff approximation (sTDA-xTB). Journal of Chemical Physics, 2016, 145, 054103.	3.0	115
15	Enantiotoposâ€Selective Cï¿½H Oxygenation Catalyzed by a Supramolecular Ruthenium Complex. Angewandte Chemie - International Edition, 2015, 54, 691-695.	13.8	98
16	Enantiomerically Pure [M₆L₁₂] or [M₁₂L₂₄] Polyhedra from Flexible Bis(Pyridine) Ligands. Angewandte Chemie - International Edition, 2014, 53, 1693-1698.	13.8	96
17	TeraChem: Accelerating electronic structure and ab initio molecular dynamics with graphical processing units. Journal of Chemical Physics, 2020, 152, 224110.	3.0	87
18	An Octanuclear Metallosupramolecular Cage Designed To Exhibit Spinâ€Crossover Behavior. Angewandte Chemie - International Edition, 2017, 56, 4930-4935.	13.8	80

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19	The Thermochemistry of London Dispersionâ€Driven Transition Metal Reactions: Getting the â€˜Right Answer for the Right Reasonâ€™. ChemistryOpen, 2014, 3, 177-189.	1.9	77
20	Photochemical Deracemization of Primary Allene Amides by Triplet Energy Transfer: A Combined Synthetic and Theoretical Study. Journal of the American Chemical Society, 2021, 143, 11209-11217.	13.7	55
21	A general intermolecular force field based on tight-binding quantum chemical calculations. Journal of Chemical Physics, 2017, 147, 161708.	3.0	53
22	Nonadiabatic Dynamics Simulation of the Wavelength-Dependent Photochemistry of Azobenzene Excited to the nÏ€* and Ï€Ï€* Excited States. Journal of the American Chemical Society, 2020, 142, 20680-20690.	13.7	46
23	Effect of Conjugation Pathway in Metal-Free Room-Temperature Dual Singletâ€“Triplet Emitters for Organic Light-Emitting Diodes. Journal of Physical Chemistry Letters, 2016, 7, 4802-4808.	4.6	42
24	Cycloadditions of Donorâ€“Acceptor Cyclopropanes and â€‹butanes using S=Nâ€Containing Reagents: Access to Cyclic Sulfinamides, Sulfonamides, and Sulfinamidines. Angewandte Chemie - International Edition, 2021, 60, 25825-25831.	13.8	40
25	From attraction to repulsion: anionâ€“Ï€ interactions between bromide and fluorinated phenyl groups. Chemical Communications, 2011, 47, 8542.	4.1	39
26	Holeâ€“hole Tammâ€“Dancoff-approximated density functional theory: A highly efficient electronic structure method incorporating dynamic and static correlation. Journal of Chemical Physics, 2020, 153, 024110.	3.0	34
27	Photochemical Deracemization of Chiral Alkenes via Triplet Energy Transfer. Journal of the American Chemical Society, 2022, 144, 10133-10138.	13.7	34
28	Biomolecular Structure Information from High-Speed Quantum Mechanical Electronic Spectra Calculation. Journal of the American Chemical Society, 2017, 139, 11682-11685.	13.7	33
29	Vollautomatisierte quantenchemische Berechnung von Spinâ€Spinâ€gekoppelten magnetischen Kernspinresonanzspektren. Angewandte Chemie, 2017, 129, 14958-14964.	2.0	32
30	Electronic Circular Dichroism of [16]Helicene With Simplified TDâ€DFT: Beyond the Single Structure Approach. Chirality, 2016, 28, 365-369.	2.6	30
31	Direct synthesis of a geminal zwitterionic phosphonium/hydridoborate system â€“ developing an alternative tool for generating frustrated Lewis pair hydrogen activation systems. Organic and Biomolecular Chemistry, 2015, 13, 5783-5792.	2.8	28
32	Ab Initio Nonadiabatic Molecular Dynamics with Holeâ€“Hole Tammâ€“Dancoff Approximated Density Functional Theory. Journal of Chemical Theory and Computation, 2020, 16, 5499-5511.	5.3	27
33	Hot exciplexes in U-shaped TADF molecules with emission from locally excited states. Nature Communications, 2021, 12, 6179.	12.8	25
34	The Association of Two â€œFrustratedâ€Lewis Pairs by Stateâ€ofâ€theâ€Art Quantum Chemical Methods. Israel Journal of Chemistry, 2015, 55, 235-242.	2.3	23
35	Electronic Circular Dichroism of Highly Conjugated Ï€-Systems: Breakdown of the Tammâ€“Dancoff/Configuration Interaction Singles Approximation. Journal of Physical Chemistry A, 2015, 119, 3653-3662.	2.5	23
36	Ein achtkerniger metallosupramolekularer WÃ¼rfel mit Spinâ€Crossoverâ€Eigenschaften. Angewandte Chemie, 2017, 129, 5012-5017.	2.0	19

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37	Diastereoselective Selfâ€Assembly of a Neutral Dinuclear Doubleâ€Stranded Zinc(II) Helicate via Narcissistic Selfâ€Sorting. Chemistry - A European Journal, 2017, 23, 12380-12386.	3.3	18
38	A Simplified Spin-Flip Time-Dependent Density Functional Theory Approach for the Electronic Excitation Spectra of Very Large Diradicals. Journal of Physical Chemistry A, 2019, 123, 5815-5825.	2.5	17
39	Pyridyl Containing 1,5-Diaza-3,7-diphosphacyclooctanes as Bridging Ligands for Dinuclear Copper(I) Complexes. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2017, 643, 895-902.	1.2	16
40	Free electrons and ionic liquids: study of excited states by means of electron-energy loss spectroscopy and the density functional theory multireference configuration interaction method. Physical Chemistry Chemical Physics, 2015, 17, 15771-15780.	2.8	14
41	Synthesis and Comprehensive Structural and Chiroptical Characterization of Enones Derived from (â^')-Î±-Santonin by Experiment and Theory. Journal of Organic Chemistry, 2016, 81, 4588-4600.	3.2	13
42	Benzimidazolylquinoxalines: novel fluorophores with tuneable sensitivity to solvent effects. Physical Chemistry Chemical Physics, 2017, 19, 6095-6104.	2.8	11
43	Chiral photochemistry of achiral molecules. Nature Communications, 2022, 13, 2091.	12.8	11
44	Enamine/butadienylborane cycloaddition in the frustrated Lewis pair regime. Organic and Biomolecular Chemistry, 2015, 13, 10477-10486.	2.8	10
45	Synthesis, Chiral Resolution, and Absolute Configuration of Functionalized TrÃ¶gerâ€™s Base Derivatives: Part III. Synthesis, 2015, 47, 3118-3132.	2.3	9
46	Recent research directions in Fribourg: nuclear dynamics in resonances revealed by 2-dimensional EEL spectra, electron collisions with ionic liquids and electronic excitation of pyrimidine. European Physical Journal D, 2016, 70, 1.	1.3	9
47	Indirect synthesis of a pair of formal methane activation products at a phosphane/borane frustrated Lewis pair. Dalton Transactions, 2016, 45, 19230-19233.	3.3	8
48	Cycloadditions of Donorâ€“Acceptor Cyclopropanes and â€butanes using S=Nâ€Containing Reagents: Access to Cyclic Sulfinamides, Sulfonamides, and Sulfinamidines. Angewandte Chemie, 2021, 133, 26029-26035.	2.0	8
49	Cover Image, Volume 11, Issue 2. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1523.	14.6	5
50	Extension of the element parameter set for ultra-fast excitation spectra calculation (sTDA-xTB). Molecular Physics, 2019, 117, 1104-1116.	1.7	4
51	Predictions of Pre-edge Features in Time-Resolved Near-Edge X-ray Absorption Fine Structure Spectroscopy from Holeâ€“Hole Tammâ€“Dancoff-Approximated Density Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 7120-7133.	5.3	3
52	Frontispiece: An Octanuclear Metallosupramolecular Cage Designed To Exhibit Spinâ€Crossover Behavior. Angewandte Chemie - International Edition, 2017, 56, .	13.8	1
53	Influence of regioisomerism in bis(terpyridine) based exciplexes with delayed fluorescence. Journal of Materials Chemistry C, 2022, 10, 7699-7706.	5.5	1
54	Frontispiz: Ein achtkerniger metallosupramolekularer WÃ¼rfel mit Spinâ€Crossoverâ€Eigenschaften. Angewandte Chemie, 2017, 129, .	2.0	0