Christoph Bannwarth

List of Publications by Citations

55 papers	4,898 citations	25 h-index	67 g-index
67 ext. papers	6,681 ext. citations	8.7 avg, IF	6.54 L-index

#	Paper	IF	Citations
55	Dispersion-Corrected Mean-Field Electronic Structure Methods. *Chemical Reviews*, **2016**, 116, 5105-54	68.1	738
54	GFN2-xTB-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	6.4	717
53	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 = 1-86). *Journal of Chemical Theory and Computation*, **2017**, 13, 1989-2009	6.4	592
52	Consistent structures and interactions by density functional theory with small atomic orbital basis sets. *Journal of Chemical Physics*, **2015**, 143, 054107	3.9	404
51	A generally applicable atomic-charge dependent London dispersion correction. *Journal of Chemical Physics*, **2019**, 150, 154122	3.9	300
50	Extension of the D3 dispersion coefficient model. *Journal of Chemical Physics*, **2017**, 147, 034112	3.9	293
49	B97-3c: A revised low-cost variant of the B97-D density functional method. *Journal of Chemical Physics*, **2018**, 148, 064104	3.9	221
48	Combinations of ethers and B(C6F5)3 function as hydrogenation catalysts. *Angewandte Chemie - International Edition*, **2013**, 52, 7492-5	16.4	160
47	Extended tight-binding quantum chemistry methods. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1493	7.9	149
46	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	138
45	Fully Automated Quantum-Chemistry-Based Computation of Spin-Spin-Coupled Nuclear Magnetic Resonance Spectra. *Angewandte Chemie - International Edition*, **2017**, 56, 14763-14769	16.4	107
44	Catalytic deracemization of chiral allenes by sensitized excitation with visible light. *Nature*, **2018**, 564, 240-243	50.4	95
43	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	3.9	87
42	Enantiomerically pure [M(6)L(12)] or [M(12)L(24)] polyhedra from flexible bis(pyridine) ligands. *Angewandte Chemie - International Edition*, **2014**, 53, 1693-8	16.4	86
41	The thermochemistry of london dispersion-driven transition metal reactions: getting the 'right answer for the right reason'. *ChemistryOpen*, **2014**, 3, 177-89	2.3	70
40	Combinations of Ethers and B(C6F5)3 Function as Hydrogenation Catalysts. *Angewandte Chemie*, **2013**, 125, 7640-7643	3.6	64
39	An Octanuclear Metallosupramolecular Cage Designed To Exhibit Spin-Crossover Behavior. *Angewandte Chemie - International Edition*, **2017**, 56, 4930-4935	16.4	59

38	TeraChem: A graphical processing unit-accelerated electronic structure package for large-scale ab initio molecular dynamics. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1494	7.9	49
37	Enantiotopos-selective C-H oxygenation catalyzed by a supramolecular ruthenium complex. *Angewandte Chemie - International Edition*, **2015**, 54, 691-5	16.4	46
36	TeraChem: Accelerating electronic structure and ab initio molecular dynamics with graphical processing units. *Journal of Chemical Physics*, **2020**, 152, 224110	3.9	40
35	From attraction to repulsion: anion-π interactions between bromide and fluorinated phenyl groups. *Chemical Communications*, **2011**, 47, 8542-4	5.8	37
34	A general intermolecular force field based on tight-binding quantum chemical calculations. *Journal of Chemical Physics*, **2017**, 147, 161708	3.9	36
33	Enantiomerenreine [M6L12]- oder [M12L24]-Polyeder aus flexiblen Bis(pyridin)-Liganden. *Angewandte Chemie*, **2014**, 126, 1719-1724	3.6	32
32	Effect of Conjugation Pathway in Metal-Free Room-Temperature Dual Singlet-Triplet Emitters for Organic Light-Emitting Diodes. *Journal of Physical Chemistry Letters*, **2016**, 7, 4802-4808	6.4	30
31	Vollautomatisierte quantenchemische Berechnung von Spin-Spin- gekoppelten magnetischen Kernspinresonanzspektren. *Angewandte Chemie*, **2017**, 129, 14958-14964	3.6	25
30	Electronic Circular Dichroism of [16]Helicene With Simplified TD-DFT: Beyond the Single Structure Approach. *Chirality*, **2016**, 28, 365-9	2.1	24
29	Biomolecular Structure Information from High-Speed Quantum Mechanical Electronic Spectra Calculation. *Journal of the American Chemical Society*, **2017**, 139, 11682-11685	16.4	24
28	Enantiotopos-selektive CH-Oxygenierung mit einem supramolekularen Ruthenium-Katalysator. *Angewandte Chemie*, **2015**, 127, 701-705	3.6	23
27	Direct synthesis of a geminal zwitterionic phosphonium/hydridoborate system--developing an alternative tool for generating frustrated Lewis pair hydrogen activation systems. *Organic and Biomolecular Chemistry*, **2015**, 13, 5783-92	3.9	22
26	The Association of Two Frustrated Lewis Pairs by State-of-the-Art Quantum Chemical Methods. *Israel Journal of Chemistry*, **2015**, 55, 235-242	3.4	20
25	Nonadiabatic Dynamics Simulation of the Wavelength-Dependent Photochemistry of Azobenzene Excited to the nπ* and π* Excited States. *Journal of the American Chemical Society*, **2020**, 142, 20680-20690	16.4	20
24	Diastereoselective Self-Assembly of a Neutral Dinuclear Double-Stranded Zinc(II) Helicate via Narcissistic Self-Sorting. *Chemistry - A European Journal*, **2017**, 23, 12380-12386	4.8	16
23	Electronic circular dichroism of highly conjugated π systems: breakdown of the Tamm-Dancoff/configuration interaction singles approximation. *Journal of Physical Chemistry A*, **2015**, 119, 3653-62	2.8	15
22	Hole-hole Tamm-Dancoff-approximated density functional theory: A highly efficient electronic structure method incorporating dynamic and static correlation. *Journal of Chemical Physics*, **2020**, 153, 024110	3.9	15
21	Ein achtkerniger metallosupramolekularer Würfel mit Spin-Crossover-Eigenschaften. *Angewandte Chemie*, **2017**, 129, 5012-5017	3.6	13

20	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, 15771-80	3.6	12
19	Nonadiabatic Molecular Dynamics with Hole-Hole Tamm-Dancoff Approximated Density Functional Theory. *Journal of Chemical Theory and Computation*, **2020**, 16, 5499-5511	6.4	12
18	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	16.4	12
17	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	1.3	11
16	Benzimidazolylquinoxalines: novel fluorophores with tuneable sensitivity to solvent effects. *Physical Chemistry Chemical Physics*, **2017**, 19, 6095-6104	3.6	10
15	Synthesis and Comprehensive Structural and Chiroptical Characterization of Enones Derived from (-)-α-Santonin by Experiment and Theory. *Journal of Organic Chemistry*, **2016**, 81, 4588-600	4.2	10
14	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	2.8	9
13	Enamine/butadienylborane cycloaddition in the frustrated Lewis pair regime. *Organic and Biomolecular Chemistry*, **2015**, 13, 10477-86	3.9	8
12	Synthesis, Chiral Resolution, and Absolute Configuration of Functionalized Tröger's Base Derivatives: Part III. *Synthesis*, **2015**, 47, 3118-3132	2.9	8
11	Indirect synthesis of a pair of formal methane activation products at a phosphane/borane frustrated Lewis pair. *Dalton Transactions*, **2016**, 45, 19230-19233	4.3	7
10	Hot exciplexes in U-shaped TADF molecules with emission from locally excited states. *Nature Communications*, **2021**, 12, 6179	17.4	7
9	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	6
8	Non-covalent Stabilization in Transition Metal Coordination and Organometallic Complexes **2016**, 115-143		4
7	Extension of the element parameter set for ultra-fast excitation spectra calculation (sTDA-xTB). *Molecular Physics*, **2019**, 117, 1104-1116	1.7	3
6	Cover Image, Volume 11, Issue 2. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1523	7.9	3
5	A Generally Applicable Atomic-Charge Dependent London Dispersion Correction Scheme		2
4	Cycloadditions of Donor-Acceptor Cyclopropanes and -butanes using S=N-Containing Reagents: Access to Cyclic Sulfinamides, Sulfonamides, and Sulfinamidines. *Angewandte Chemie - International Edition*, **2021**, 60, 25825-25831	16.4	2
3	Frontispiece: An Octanuclear Metallosupramolecular Cage Designed To Exhibit Spin-Crossover Behavior. *Angewandte Chemie - International Edition*, **2017**, 56,	16.4	1

2	Chiral photochemistry of achiral molecules.. *Nature Communications*, **2022**, 13, 2091	17.4	1
1	Predictions of Pre-edge Features in Time-Resolved Near-Edge X-ray Absorption Fine Structure Spectroscopy from Hole-Hole Tamm-Dancoff-Approximated Density Functional Theory. *Journal of Chemical Theory and Computation*, **2021**, 17, 7120-7133	6.4	0