Christoph Bannwarth

List of Publications by Year
in descending order

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Version: 2024-02-01

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	Chiral photochemistry of achiral molecules. Nature Communications, 2022, 13, 2091.	12.8	11
2	Influence of regioisomerism in bis(terpyridine) based exciplexes with delayed fluorescence. Journal of Materials Chemistry C, 2022, 10, 7699-7706.	5.5	1
3	Photochemical Deracemization of Chiral Alkenes via Triplet Energy Transfer. Journal of the American Chemical Society, 2022, 144, 10133-10138.	13.7	34
4	Extended <scp>tightâ€binding</scp> quantum chemistry methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1493.	14.6	596
5	<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
6	Cover Image, Volume 11, Issue 2. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1523.	14.6	5
7	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
8	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
9	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
10	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
11	Hot exciplexes in U-shaped TADF molecules with emission from locally excited states. Nature Communications, 2021, 12, 6179.	12.8	25
12	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
13	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
14	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
15	TeraChem: Accelerating electronic structure and ab initio molecular dynamics with graphical processing units. Journal of Chemical Physics, 2020, 152, 224110.	3.0	87
16	Extension of the element parameter set for ultra-fast excitation spectra calculation (sTDA-xTB). Molecular Physics, 2019, 117, 1104-1116.	1.7	4
17	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
18	A generally applicable atomic-charge dependent London dispersion correction. Journal of Chemical Physics, 2019, 150, 154122.	3.0	697

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19	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
20	B97-3c: A revised low-cost variant of the B97-D density functional method. Journal of Chemical Physics, 2018, 148, 064104.	3.0	400
21	Catalytic deracemization of chiral allenes by sensitized excitation with visible light. Nature, 2018, 564, 240-243.	27.8	180
22	Benzimidazolylquinoxalines: novel fluorophores with tuneable sensitivity to solvent effects. Physical Chemistry Chemical Physics, 2017, 19, 6095-6104.	2.8	11
23	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
24	Ein achtkerniger metallosupramolekularer WÃ¼rfel mit Spinâ€Crossoverâ€Eigenschaften. Angewandte Chemie, 2017, 129, 5012-5017.	2.0	19
25	Frontispiece: An Octanuclear Metallosupramolecular Cage Designed To Exhibit Spinâ€Crossover Behavior. Angewandte Chemie - International Edition, 2017, 56, .	13.8	1
26	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
27	An Octanuclear Metallosupramolecular Cage Designed To Exhibit Spinâ€Crossover Behavior. Angewandte Chemie - International Edition, 2017, 56, 4930-4935.	13.8	80
28	Vollautomatisierte quantenchemische Berechnung von Spinâ€Spinâ€gekoppelten magnetischen Kernspinresonanzspektren. Angewandte Chemie, 2017, 129, 14958-14964.	2.0	32
29	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
30	A general intermolecular force field based on tight-binding quantum chemical calculations. Journal of Chemical Physics, 2017, 147, 161708.	3.0	53
31	Extension of the D3 dispersion coefficient model. Journal of Chemical Physics, 2017, 147, 034112.	3.0	617
32	Frontispiz: Ein achtkerniger metallosupramolekularer WÃ¼rfel mit Spinâ€Crossoverâ€Eigenschaften. Angewandte Chemie, 2017, 129, .	2.0	0
33	Biomolecular Structure Information from High-Speed Quantum Mechanical Electronic Spectra Calculation. Journal of the American Chemical Society, 2017, 139, 11682-11685.	13.7	33
34	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
35	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
36	Dispersion-Corrected Mean-Field Electronic Structure Methods. Chemical Reviews, 2016, 116, 5105-5154.	47.7	1,032

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37	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
38	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
39	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
40	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
41	Electronic Circular Dichroism of [16]Helicene With Simplified TDâ€DFT: Beyond the Single Structure Approach. Chirality, 2016, 28, 365-369.	2.6	30
42	Enantiotoposâ€Selective Cï£¿H Oxygenation Catalyzed by a Supramolecular Ruthenium Complex. Angewandte Chemie - International Edition, 2015, 54, 691-695.	13.8	98
43	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
44	Synthesis, Chiral Resolution, and Absolute Configuration of Functionalized TrÃ¶ger's Base Derivatives: Part III. Synthesis, 2015, 47, 3118-3132.	2.3	9
45	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
46	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
47	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
48	Consistent structures and interactions by density functional theory with small atomic orbital basis sets. Journal of Chemical Physics, 2015, 143, 054107.	3.0	605
49	Enamine/butadienylborane cycloaddition in the frustrated Lewis pair regime. Organic and Biomolecular Chemistry, 2015, 13, 10477-10486.	2.8	10
50	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
51	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
52	Enantiomerically Pure [M₆L₁₂] or [M₁₂L₂₄] Polyhedra from Flexible Bis(Pyridine) Ligands. Angewandte Chemie - International Edition, 2014, 53, 1693-1698.	13.8	96
53	Combinations of Ethers and B(C₆F₅)₃ Function as Hydrogenation Catalysts. Angewandte Chemie - International Edition, 2013, 52, 7492-7495.	13.8	180
54	From attraction to repulsion: anionâ€"Ï€ interactions between bromide and fluorinated phenyl groups. Chemical Communications, 2011, 47, 8542.	4.1	39