Sebastian Ehlert

List of Publications by Year
in descending order

300 papers	111,326 citations	7069 78 h-index	261 299 g-index
312 all docs	312 docs citations	312 times ranked	65687 citing authors

#	Article	IF	Citations
1	A consistent and accurateab initioparametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. Journal of Chemical Physics, 2010, 132, 154104.	1.2	35,972
2	Semiempirical GGA-type density functional constructed with a long-range dispersion correction. Journal of Computational Chemistry, 2006, 27, 1787-1799.	1.5	24,222
3	Effect of the damping function in dispersion corrected density functional theory. Journal of Computational Chemistry, 2011, 32, 1456-1465.	1.5	15,980
4	Semiempirical hybrid density functional with perturbative second-order correlation. Journal of Chemical Physics, 2006, 124, 034108.	1.2	2,729
5	Density functional theory with London dispersion corrections. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 211-228.	6.2	2,030
6	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.	2.3	1,704
7	Supramolecular Binding Thermodynamics by Dispersionâ€Corrected Density Functional Theory. Chemistry - A European Journal, 2012, 18, 9955-9964.	1.7	1,346
8	A look at the density functional theory zoo with the advanced GMTKN55 database for general main group thermochemistry, kinetics and noncovalent interactions. Physical Chemistry Chemical Physics, 2017, 19, 32184-32215.	1.3	1,230
9	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.	2.3	1,072
10	Dispersion-Corrected Mean-Field Electronic Structure Methods. Chemical Reviews, 2016, 116, 5105-5154.	23.0	1,032
11	Automated exploration of the low-energy chemical space with fast quantum chemical methods. Physical Chemistry Chemical Physics, 2020, 22, 7169-7192.	1.3	966
12	Do Special Noncovalent Ï€â€“Ï€ Stacking Interactions Really Exist?. Angewandte Chemie - International Edition, 2008, 47, 3430-3434.	7.2	928
13	A generally applicable atomic-charge dependent London dispersion correction. Journal of Chemical Physics, 2019, 150, 154122.	1.2	697
14	Extension of the D3 dispersion coefficient model. Journal of Chemical Physics, 2017, 147, 034112.	1.2	617
15	Consistent structures and interactions by density functional theory with small atomic orbital basis sets. Journal of Chemical Physics, 2015, 143, 054107.	1.2	605
16	Extended <scp>tightâ€binding</scp> quantum chemistry methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1493.	6.2	596
17	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. Journal of Chemical Physics, 2020, 152, 124101.	1.2	589
18	Rapid intramolecular heterolytic dihydrogen activation by a four-membered heterocyclic phosphaneâ€“borane adduct. Chemical Communications, 2007, , 5072.	2.2	563

#	Article	IF	Citations
19	A geometrical correction for the inter- and intra-molecular basis set superposition error in Hartree-Fock and density functional theory calculations for large systems. Journal of Chemical Physics, 2012, 136, 154101.	1.2	556
20	Exploration of Chemical Compound, Conformer, and Reaction Space with Meta-Dynamics Simulations Based on Tight-Binding Quantum Chemical Calculations. Journal of Chemical Theory and Computation, 2019, 15, 2847-2862.	2.3	551
21	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
22	DFT-D3 Study of Some Molecular Crystals. Journal of Physical Chemistry C, 2014, 118, 7615-7621.	1.5	457
23	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	0.5	445
24	B97-3c: A revised low-cost variant of the B97-D density functional method. Journal of Chemical Physics, 2018, 148, 064104.	1.2	400
25	The Mechanism of Dihydrogen Activation by Frustrated Lewis Pairs Revisited. Angewandte Chemie - International Edition, 2010, 49, 1402-1405.	7.2	394
26	A General Database for Main Group Thermochemistry, Kinetics, and Noncovalent Interactions â^' Assessment of Common and Reparameterized (meta-)GGA Density Functionals. Journal of Chemical Theory and Computation, 2010, 6, 107-126.	2.3	389
27	Benchmarking of London Dispersion-Accounting Density Functional Theory Methods on Very Large Molecular Complexes. Journal of Chemical Theory and Computation, 2013, 9, 1580-1591.	2.3	362
28	Corrected small basis set Hartreeâ€Fock method for large systems. Journal of Computational Chemistry, 2013, 34, 1672-1685.	1.5	358
29	Systemâ€Dependent Dispersion Coefficients for the DFTâ€D3 Treatment of Adsorption Processes on Ionic Surfaces. ChemPhysChem, 2011, 12, 3414-3420.	1.0	318
30	Doubleâ€hybrid density functionals. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 576-600.	6.2	292
31	r2SCAN-3c: A â€œSwiss army knifeâ€•composite electronic-structure method. Journal of Chemical Physics, 2021, 154, 064103.	1.2	290
32	Benchmarking Density Functional Methods against the S66 and S66x8 Datasets for Nonâ€Covalent Interactions. ChemPhysChem, 2011, 12, 3421-3433.	1.0	283
33	Full Selectivity Control in Cobalt(III)â€Catalyzed Câ^'H Alkylations by Switching of the Câ^'H Activation Mechanism. Angewandte Chemie - International Edition, 2017, 56, 10378-10382.	7.2	243
34	A simplified Tamm-Dancoff density functional approach for the electronic excitation spectra of very large molecules. Journal of Chemical Physics, 2013, 138, 244104.	1.2	242
35	Effects of London dispersion correction in density functional theory on the structures of organic molecules in the gas phase. Physical Chemistry Chemical Physics, 2013, 15, 16031.	1.3	238
36	Steric Crowding Can Stabilize a Labile Molecule: Solving the Hexaphenylethane Riddle. Angewandte Chemie - International Edition, 2011, 50, 12639-12642.	7.2	232

#	Article	IF	Citations
37	Robust Atomistic Modeling of Materials, Organometallic, and Biochemical Systems. Angewandte Chemie - International Edition, 2020, 59, 15665-15673.	7.2	224
38	â€œMindlessâ€•DFT Benchmarking. Journal of Chemical Theory and Computation, 2009, 5, 993-1003.	2.3	215
39	Performance of the van der Waals Density Functional VV10 and (hybrid)GGA Variants for Thermochemistry and Noncovalent Interactions. Journal of Chemical Theory and Computation, 2011, 7, 3866-3871.	2.3	213
40	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.	1.1	211
41	Performance of dispersion-corrected density functional theory for the interactions in ionic liquids. Physical Chemistry Chemical Physics, 2012, 14, 4875.	1.3	202
42	Comprehensive Thermochemical Benchmark Set of Realistic Closed-Shell Metal Organic Reactions. Journal of Chemical Theory and Computation, 2018, 14, 2596-2608.	2.3	202
43	Assessment of Orbital-Optimized, Spin-Component Scaled Second-Order Many-Body Perturbation Theory for Thermochemistry and Kinetics. Journal of Chemical Theory and Computation, 2009, 5, 3060-3073.	2.3	199
44	Spinâ€componentâ€scaled electron correlation methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 886-906.	6.2	197
45	A Practicable Realâ€Space Measure and Visualization of Static Electronâ€Correlation Effects. Angewandte Chemie - International Edition, 2015, 54, 12308-12313.	7.2	194
46	Comprehensive Benchmark of Association (Free) Energies of Realistic Hostâ€“Guest Complexes. Journal of Chemical Theory and Computation, 2015, 11, 3785-3801.	2.3	188
47	Robust and Efficient Implicit Solvation Model for Fast Semiempirical Methods. Journal of Chemical Theory and Computation, 2021, 17, 4250-4261.	2.3	186
48	Reaction of Frustrated Lewis Pairs with Conjugated Ynonesâ€Selective Hydrogenation of the Carbonâ€“Carbon Triple Bond. Angewandte Chemie - International Edition, 2011, 50, 7183-7186.	7.2	169
49	Is Spin-Component Scaled Second-Order MÃllerâ^'Plesset Perturbation Theory an Appropriate Method for the Study of Noncovalent Interactions in Molecules?. Journal of Physical Chemistry A, 2007, 111, 4862-4868.	1.1	164
50	Fully Automated Quantumâ€Chemistryâ€Based Computation of Spinâ€“Spinâ€Coupled Nuclear Magnetic Resonance Spectra. Angewandte Chemie - International Edition, 2017, 56, 14763-14769.	7.2	158
51	Accurate Modeling of Organic Molecular Crystals by Dispersion-Corrected Density Functional Tight Binding (DFTB). Journal of Physical Chemistry Letters, 2014, 5, 1785-1789.	2.1	155
52	A General Quantum Mechanically Derived Force Field (QMDFF) for Molecules and Condensed Phase Simulations. Journal of Chemical Theory and Computation, 2014, 10, 4497-4514.	2.3	154
53	Reactions of phosphorus/boron frustrated Lewis pairs with SO₂. Chemical Science, 2013, 4, 213-219.	3.7	150
54	Towards First Principles Calculation of Electron Impact Mass Spectra of Molecules. Angewandte Chemie - International Edition, 2013, 52, 6306-6312.	7.2	148

#	Article	IF	Citations
55	Benchmark Study of the Performance of Density Functional Theory for Bond Activations with (Ni,Pd)â€Based Transitionâ€Metal Catalysts. ChemistryOpen, 2013, 2, 115-124.	0.9	146
56	Computational Chemistry: The Fate of Current Methods and Future Challenges. Angewandte Chemie - International Edition, 2018, 57, 4170-4176.	7.2	138
57	Extension and evaluation of the D4 London-dispersion model for periodic systems. Physical Chemistry Chemical Physics, 2020, 22, 8499-8512.	1.3	138
58	Frustrated Lewis Pair Catalyzed Dehydrogenative Oxidation of Indolines and Other Heterocycles. Angewandte Chemie - International Edition, 2016, 55, 12219-12223.	7.2	129
59	Cationâ^'Cation â€œAttractionâ€: When London Dispersion Attraction Wins over Coulomb Repulsion. Inorganic Chemistry, 2011, 50, 2619-2628.	1.9	127
60	Formation of Cyclic Allenes and Cumulenes by Cooperative Addition of Frustrated Lewis Pairs to Conjugated Enynes and Diynes. Angewandte Chemie - International Edition, 2010, 49, 2414-2417.	7.2	125
61	Understanding and Quantifying London Dispersion Effects in Organometallic Complexes. Accounts of Chemical Research, 2019, 52, 258-266.	7.6	117
62	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.	1.2	115
63	Efficient Quantum Chemical Calculation of Structure Ensembles and Free Energies for Nonrigid Molecules. Journal of Physical Chemistry A, 2021, 125, 4039-4054.	1.1	105
64	The Fractional Occupation Number Weighted Density as a Versatile Analysis Tool for Molecules with a Complicated Electronic Structure. Chemistry - A European Journal, 2017, 23, 6150-6164.	1.7	102
65	Catalytic Ketone Hydrodeoxygenation Mediated by Highly Electrophilic Phosphonium Cations. Angewandte Chemie - International Edition, 2015, 54, 8250-8254.	7.2	100
66	Mild Cobalt(III)â€Catalyzed Allylative Câ^'F/Câ^'H Functionalizations at Room Temperature. Chemistry - A European Journal, 2017, 23, 12145-12148.	1.7	95
67	1,1â€Hydroboration and a Borane Adduct of Diphenyldiazomethane: A Potential Prelude to FLPâ€N₂ Chemistry. Angewandte Chemie - International Edition, 2017, 56, 16588-16592.	7.2	93
68	Copper-Catalyzed Cross-Coupling of Silicon Pronucleophiles with Unactivated Alkyl Electrophiles Coupled with Radical Cyclization. Journal of the American Chemical Society, 2016, 138, 14222-14225.	6.6	92
69	Performance of Non-Local and Atom-Pairwise Dispersion Corrections to DFT for Structural Parameters of Molecules with Noncovalent Interactions. Journal of Chemical Theory and Computation, 2013, 9, 308-315.	2.3	91
70	Quantum Chemical Benchmark Study on 46 RNA Backbone Families Using a Dinucleotide Unit. Journal of Chemical Theory and Computation, 2015, 11, 4972-4991.	2.3	90
71	How to Compute Electron Ionization Mass Spectra from First Principles. Journal of Physical Chemistry A, 2016, 120, 3755-3766.	1.1	88
72	Functional Mechanically Interlocked Molecules: Asymmetric Organocatalysis with a Catenated Bifunctional BrÃ¸nsted Acid. Angewandte Chemie - International Edition, 2017, 56, 11456-11459.	7.2	88

#	Article	IF	Citations
73	Exploration of the Solid-State Sorption Properties of Shape-Persistent Macrocyclic Nanocarbons as Bulk Materials and Small Aggregates. Journal of the American Chemical Society, 2020, 142, 8763-8775.	6.6	86
74	Benchmarking DFT and semiempirical methods on structures and lattice energies for ten ice polymorphs. Journal of Chemical Physics, 2015, 142, 124104.	1.2	84
75	Calculation of absolute molecular entropies and heat capacities made simple. Chemical Science, 2021, 12, 6551-6568.	3.7	83
76	Remarkable coordination behavior of alkyl isocyanides toward unsaturated vicinal frustrated P/B Lewis pairs. Chemical Science, 2013, 4, 2657.	3.7	81
77	N-Heterocyclic carbene (NHC) catalyzed chemoselective acylation of alcohols in the presence of amines with various acylating reagents. Chemical Science, 2013, 4, 2177.	3.7	80
78	Low-Cost Quantum Chemical Methods for Noncovalent Interactions. Journal of Physical Chemistry Letters, 2014, 5, 4275-4284.	2.1	80
79	B(C₆F₅)₃â€Catalyzed Transfer of Dihydrogen from One Unsaturated Hydrocarbon to Another. Angewandte Chemie - International Edition, 2015, 54, 12158-12162.	7.2	80
80	An Octanuclear Metallosupramolecular Cage Designed To Exhibit Spinâ€Crossover Behavior. Angewandte Chemie - International Edition, 2017, 56, 4930-4935.	7.2	80
81	Quantum chemical calculation of electron ionization mass spectra for general organic and inorganic molecules. Chemical Science, 2017, 8, 4879-4895.	3.7	79
82	Hydrosilylation of Ketones, Imines and Nitriles Catalysed by Electrophilic Phosphonium Cations: Functional Group Selectivity and Mechanistic Considerations. Chemistry - A European Journal, 2015, 21, 6491-6500.	1.7	78
83	The Thermochemistry of London Dispersionâ€Driven Transition Metal Reactions: Getting the â€˜Right Answer for the Right Reasonâ€™. ChemistryOpen, 2014, 3, 177-189.	0.9	77
84	Blind Prediction of Binding Affinities for Charged Supramolecular Hostâ€“Guest Systems: Achievements and Shortcomings of DFT-D3. Journal of Physical Chemistry B, 2014, 118, 3431-3440.	1.2	77
85	Assessing Density Functional Theory for Chemically Relevant Open-Shell Transition Metal Reactions. Journal of Chemical Theory and Computation, 2021, 17, 6134-6151.	2.3	75
86	Dispersion Corrected Hartreeâ€“Fock and Density Functional Theory for Organic Crystal Structure Prediction. Topics in Current Chemistry, 2013, 345, 1-23.	4.0	72
87	Frustrated Lewis Pairâ€Catalyzed Cycloisomerization of 1,5â€Enynes via a 5â€endoâ€dig Cyclization/Protodeborylation Sequence. Angewandte Chemie - International Edition, 2016, 55, 4336-4339.	7.2	72
88	Structure Optimisation of Large Transitionâ€Metal Complexes with Extended Tightâ€Binding Methods. Angewandte Chemie - International Edition, 2019, 58, 11078-11087.	7.2	72
89	Comparative Theoretical Study on Charge-Transfer Fluorescence Probes:Â 6-Propanoyl-2-(N,N-dimethylamino)naphthalene and Derivatives. Journal of Physical Chemistry A, 1998, 102, 7149-7156.	1.1	70
90	Frustrated Lewis Pair Catalyzed Hydrogenation of Amides: Halides as Active Lewis Base in the Metal-Free Hydrogen Activation. Journal of the American Chemical Society, 2019, 141, 159-162.	6.6	70

#	Article	IF	Citations
91	r2SCAN-D4: Dispersion corrected meta-generalized gradient approximation for general chemical applications. Journal of Chemical Physics, 2021, 154, 061101.	1.2	70
92	Titanoceneâ€Catalyzed Radical Opening of Nâ€Acylated Aziridines. Angewandte Chemie - International Edition, 2017, 56, 12654-12657.	7.2	67
93	A diuranium carbide cluster stabilized inside a C80 fullerene cage. Nature Communications, 2018, 9, 2753.	5.8	63
94	BNB-Doped Phenalenyls: Modular Synthesis, Optoelectronic Properties, and One-Electron Reduction. Journal of the American Chemical Society, 2020, 142, 11072-11083.	6.6	63
95	Intramolecular London Dispersion Interaction Effects on Gas-Phase and Solid-State Structures of Diamondoid Dimers. Journal of the American Chemical Society, 2017, 139, 16696-16707.	6.6	62
96	HYDROPHOBE Challenge: A Joint Experimental and Computational Study on the Hostâ€“Guest Binding of Hydrocarbons to Cucurbiturils, Allowing Explicit Evaluation of Guest Hydration Free-Energy Contributions. Journal of Physical Chemistry B, 2017, 121, 11144-11162.	1.2	62
97	Câ^'F Bond Activation by Silylium Cation/Phosphine Frustrated Lewis Pairs: Monoâ€Hydrodefluorination of PhCF₃, PhCF₂H and Ph₂CF₂. Chemistry - A European Journal, 2017, 23, 17692-17696.	1.7	60
98	Semiautomated Transition State Localization for Organometallic Complexes with Semiempirical Quantum Chemical Methods. Journal of Chemical Theory and Computation, 2020, 16, 2002-2012.	2.3	60
99	Highly Active Titanocene Catalysts for Epoxide Hydrosilylation: Synthesis, Theory, Kinetics, EPR Spectroscopy. Angewandte Chemie - International Edition, 2016, 55, 7671-7675.	7.2	57
100	Heterobifunctional Rotaxanes for Asymmetric Catalysis. Angewandte Chemie - International Edition, 2020, 59, 5102-5107.	7.2	56
101	A computationally efficient double hybrid density functional based on the random phase approximation. Physical Chemistry Chemical Physics, 2016, 18, 20926-20937.	1.3	55
102	HFIPâ€Assisted Single Câ^'F Bond Activation of Trifluoromethyl Ketones using Visibleâ€Light Photoredox Catalysis. Angewandte Chemie - International Edition, 2022, 61, .	7.2	54
103	Organic crystal polymorphism: a benchmark for dispersion-corrected mean-field electronic structure methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 502-513.	0.5	53
104	A general intermolecular force field based on tight-binding quantum chemical calculations. Journal of Chemical Physics, 2017, 147, 161708.	1.2	53
105	Theoretical study on conformational energies of transition metal complexes. Physical Chemistry Chemical Physics, 2021, 23, 287-299.	1.3	52
106	CO-Reduction Chemistry: Reaction of a CO-Derived Formylhydridoborate with Carbon Monoxide, with Carbon Dioxide, and with Dihydrogen. Journal of the American Chemical Society, 2017, 139, 6474-6483.	6.6	50
107	Boraneâ€Catalyzed Synthesis of Quinolines Bearing Tetrasubstituted Stereocenters by Hydride Abstractionâ€Induced Electrocyclization. Chemistry - A European Journal, 2018, 24, 16287-16291.	1.7	50
108	High accuracy quantum-chemistry-based calculation and blind prediction of macroscopic pKa values in the context of the SAMPL6 challenge. Journal of Computer-Aided Molecular Design, 2018, 32, 1139-1149.	1.3	50

#	Article	IF	Citations
109	Screened exchange hybrid density functional for accurate and efficient structures and interaction energies. Physical Chemistry Chemical Physics, 2016, 18, 15519-15523.	1.3	49
110	Automated and efficient quantum chemical determination and energetic ranking of molecular protonation sites. Journal of Computational Chemistry, 2017, 38, 2618-2631.	1.5	49
111	Efficient Computation of Free Energy Contributions for Association Reactions of Large Molecules. Journal of Physical Chemistry Letters, 2020, 11, 6606-6611.	2.1	49
112	Single-Point Hessian Calculations for Improved Vibrational Frequencies and Rigid-Rotor-Harmonic-Oscillator Thermodynamics. Journal of Chemical Theory and Computation, 2021, 17, 1701-1714.	2.3	49
113	Implementation of nuclear gradients of rangeâ€separated hybrid density functionals and benchmarking on rotational constants for organic molecules. Journal of Computational Chemistry, 2014, 35, 1509-1516.	1.5	48
114	The frustrated Lewis pair pathway to methylene phosphonium systems. Chemical Science, 2014, 5, 797-803.	3.7	47
115	Lithium Dicyclohexylamide in Transition-Metal-Free Fischerâ€“Tropsch Chemistry. Journal of the American Chemical Society, 2021, 143, 634-638.	6.6	47
116	Selective Oxidation of an Active Intramolecular Amine/Borane Frustrated Lewis Pair with Dioxygen. Journal of the American Chemical Society, 2016, 138, 4302-4305.	6.6	46
117	Towards full Quantumâ€Mechanicsâ€based Proteinâ€“Ligand Binding Affinities. ChemPhysChem, 2017, 18, 898-905.	1.0	46
118	From Additivity to Cooperativity in Chemistry: Can Cooperativity Be Measured?. Chemistry - A European Journal, 2017, 23, 5864-5873.	1.7	46
119	The Chiral Trimer and a Metastable Chiral Dimer of Achiral Hexafluoroisopropanol: A Multiâ€Messenger Study. Angewandte Chemie - International Edition, 2019, 58, 5080-5084.	7.2	46
120	Benchmark Study of Electrochemical Redox Potentials Calculated with Semiempirical and DFT Methods. Journal of Physical Chemistry A, 2020, 124, 7166-7176.	1.1	45
121	Automated Molecular Cluster Growing for Explicit Solvation by Efficient Force Field and Tight Binding Methods. Journal of Chemical Theory and Computation, 2022, 18, 3174-3189.	2.3	45
122	The furan microsolvation blind challenge for quantum chemical methods: First steps. Journal of Chemical Physics, 2018, 148, 014301.	1.2	44
123	Noncovalent Metalâ‹¯Metal Interactions: The Crucial Role of London Dispersion in a Bimetallic Indenyl System. Journal of the American Chemical Society, 2009, 131, 14156-14157.	6.6	43
124	Raising the Bar in Aromatic Donorâ€“Acceptor Interactions with Cyclic Trinuclear Gold(I) Complexes as Strong Ï€-Donors. Journal of the American Chemical Society, 2018, 140, 17932-17944.	6.6	43
125	Amideâ€Substituted Titanocenes in Hydrogenâ€Atom Transfer Catalysis. Angewandte Chemie - International Edition, 2016, 55, 1523-1526.	7.2	42
126	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.	2.1	42

#	Article	IF	Citations
127	Fast and Reasonable Geometry Optimization of Lanthanoid Complexes with an Extended Tight Binding Quantum Chemical Method. Inorganic Chemistry, 2017, 56, 12485-12491.	1.9	41
128	Nonlinear-response properties in a simplified time-dependent density functional theory (sTD-DFT) framework: Evaluation of the first hyperpolarizability. Journal of Chemical Physics, 2018, 149, 024108.	1.2	41
129	Evidence of a Donorâ€“Acceptor (Irâ€“H)â†’SiR₃ Interaction in a Trapped Ir(III) Silane Catalytic Intermediate. Organometallics, 2016, 35, 2207-2223.	1.1	40
130	Robust Atomistic Modeling of Materials, Organometallic, and Biochemical Systems. Angewandte Chemie, 2020, 132, 15795-15803.	1.6	40
131	Accurate Computation of Structures and Strain Energies of Cyclophanes with Modern DFT Methods. Israel Journal of Chemistry, 2012, 52, 180-192.	1.0	38
132	Finding the best density functional approximation to describe interaction energies and structures of ionic liquids in molecular dynamics studies. Journal of Chemical Physics, 2018, 148, 193835.	1.2	38
133	Accurate Theoretical Description of the ¹L_a and ¹L_b Excited States in Acenes Using the All Order Constricted Variational Density Functional Theory Method and the Local Density Approximation. Journal of Chemical Theory and Computation, 2012, 8, 4434-4440.	2.3	37
134	Why Does the Intramolecular Trimethyleneâ€Bridged Frustrated Lewis Pair Mes₂PCH₂CH₂CH₂B(C₆F₅)₂ Not Activate Dihydrogen?. Chemistry - A European Journal, 2016, 22, 5988-5995.	1.7	37
135	S_N2 Reactions at Tertiary Carbon Centers in Epoxides. Angewandte Chemie - International Edition, 2017, 56, 9719-9722.	7.2	37
136	Electrophilic Phosphonium Cationâ€Mediated Phosphane Oxide Reduction Using Oxalyl Chloride and Hydrogen. Angewandte Chemie - International Edition, 2018, 57, 15253-15256.	7.2	37
137	Synthesis and Dynamics of Nanosized Phenyleneâ€“Ethyleneâ€“Butadiynylene Rotaxanes and the Role of Shape Persistence. Angewandte Chemie - International Edition, 2016, 55, 3328-3333.	7.2	36
138	Intermolecular Redoxâ€Neutral Amine Cα–H Functionalization Induced by the Strong Boron Lewis Acid B(C₆F₅)₃ in the Frustrated Lewis Pair Regime. Chemistry - A European Journal, 2017, 23, 4723-4729.	1.7	36
139	Oxâ€SLIM: Synthesis of and Siteâ€Specific Labelling with a Highly Hydrophilic Trityl Spin Label. Chemistry - A European Journal, 2021, 27, 5292-5297.	1.7	36
140	Functional Mechanically Interlocked Molecules: Asymmetric Organocatalysis with a Catenated Bifunctional BrÃ¸nsted Acid. Angewandte Chemie, 2017, 129, 11614-11617.	1.6	35
141	Solid state frustrated Lewis pair chemistry. Chemical Science, 2018, 9, 4859-4865.	3.7	35
142	Coâ€“C Bond Dissociation Energies in Cobalamin Derivatives and Dispersion Effects: Anomaly or Just Challenging?. Journal of Chemical Theory and Computation, 2015, 11, 1037-1045.	2.3	34
143	Double FLP-Alkyne Exchange Reactions: A Facile Route to Te/B Heterocycles. Journal of the American Chemical Society, 2015, 137, 13264-13267.	6.6	34
144	Hydrogenation and Transfer Hydrogenation Promoted by Tethered Ruα–S Complexes: From Cooperative Dihydrogen Activation to Hydride Abstraction/Proton Release from Dihydrogen Surrogates. Chemistry - A European Journal, 2016, 22, 10009-10016.	1.7	34

#	Article	IF	Citations
145	S(<scp>vi</scp>) Lewis acids: fluorosulfoxonium cations. Chemical Communications, 2016, 52, 12418-12421.	2.2	34
146	Reactions of Boron-Derived Radicals with Nucleophiles. Journal of the American Chemical Society, 2017, 139, 426-435.	6.6	34
147	Biomolecular Structure Information from High-Speed Quantum Mechanical Electronic Spectra Calculation. Journal of the American Chemical Society, 2017, 139, 11682-11685.	6.6	33
148	Calculation of Electron Ionization Mass Spectra with Semiempirical GFNn-xTB Methods. ACS Omega, 2019, 4, 15120-15133.	1.6	33
149	Quantum Chemical Calculation of Molecular and Periodic Peptide and Protein Structures. Journal of Physical Chemistry B, 2020, 124, 3636-3646.	1.2	33
150	Vollautomatisierte quantenchemische Berechnung von Spinâ€Spinâ€•gekoppelten magnetischen Kernspinresonanzspektren. Angewandte Chemie, 2017, 129, 14958-14964.	1.6	32
151	Formation of macrocyclic ring systems by carbonylation of trifunctional P/B/B frustrated Lewis pairs. Chemical Science, 2018, 9, 1544-1550.	3.7	32
152	Electrophilic Formylation of Arenes by Silylium Ion Mediated Activation of Carbon Monoxide. Angewandte Chemie - International Edition, 2018, 57, 8301-8305.	7.2	32
153	Comprehensive Assessment of GFN Tight-Binding and Composite Density Functional Theory Methods for Calculating Gas-Phase Infrared Spectra. Journal of Chemical Theory and Computation, 2020, 16, 7044-7060.	2.3	32
154	Efficient Calculation of Small Molecule Binding in Metalâ€“Organic Frameworks and Porous Organic Cages. Journal of Physical Chemistry C, 2020, 124, 27529-27541.	1.5	32
155	Modeling of spinâ€“spin distance distributions for nitroxide labeled biomacromolecules. Physical Chemistry Chemical Physics, 2020, 22, 24282-24290.	1.3	32
156	Dispersion corrected r2SCAN based global hybrid functionals: r2SCANh, r2SCAN0, and r2SCAN50. Journal of Chemical Physics, 2022, 156, 134105.	1.2	32
157	Exploring the chemical nature of super-heavy main-group elements by means of efficient plane-wave density-functional theory. Physical Chemistry Chemical Physics, 2019, 21, 18048-18058.	1.3	31
158	Benchmarking London dispersion corrected density functional theory for noncovalent ionâ€“Ï€ interactions. Physical Chemistry Chemical Physics, 2021, 23, 11635-11648.	1.3	31
159	Electronic Circular Dichroism of [16]Helicene With Simplified TDâ€ĐFT: Beyond the Single Structure Approach. Chirality, 2016, 28, 365-369.	1.3	30
160	From QCEIMS to QCxMS: A Tool to Routinely Calculate CID Mass Spectra Using Molecular Dynamics. Journal of the American Society for Mass Spectrometry, 2021, 32, 1735-1751.	1.2	30
161	Frustrated Lewis pair addition to conjugated diynes: Formation of zwitterionic 1,2,3-butatriene derivatives. Dalton Transactions, 2012, 41, 9135.	1.6	29
162	Predicting Elastic Properties of Î²-HMX from First-Principles Calculations. Journal of Physical Chemistry B, 2015, 119, 5896-5903.	1.2	29

#	Article	IF	Citations
163	Rapid Dihydrogen Cleavage by Persistent Nitroxide Radicals under Frustrated Lewis Pair Conditions. Chemistry - A European Journal, 2016, 22, 9504-9507.	1.7	29
164	Counterintuitive Interligand Angles in the Diaryls E{C₆H₃-2,6-(C₆H₂-2,4,6-ⁱPr₃)₂}<sub (E = Ge, Sn, or Pb) and Related Species: The Role of London Dispersion Forces. Organometallics, 2018, 37, 2075-2085.	1.1	29
165	Aggregation Behavior of a Sixâ€Membered Cyclic Frustrated Phosphane/Borane Lewis Pair: Formation of a Supramolecular Cyclooctameric Macrocyclic Ring System. Angewandte Chemie - International Edition, 2019, 58, 882-886.	7.2	29
166	Chiral Dibenzopentaleneâ€Based Conjugated Nanohoops through Stereoselective Synthesis. Angewandte Chemie - International Edition, 2021, 60, 10680-10689.	7.2	29
167	Automated Quantum Chemistry Based Molecular Dynamics Simulations of Electron Ionization Induced Fragmentations of the Nucleobases Uracil, Thymine, Cytosine, and Guanine. European Journal of Mass Spectrometry, 2015, 21, 125-140.	0.5	28
168	Coupling of Carbon Monoxide with Nitrogen Monoxide at a Frustrated Lewis Pair Template. Angewandte Chemie - International Edition, 2016, 55, 9216-9219.	7.2	28
169	The first microsolvation step for furans: New experiments and benchmarking strategies. Journal of Chemical Physics, 2020, 152, 164303.	1.2	28
170	Halogen bonded supramolecular capsules: a challenging test case for quantum chemical methods. Chemical Communications, 2016, 52, 9893-9896.	2.2	26
171	Reversible formylborane/SO₂coupling at a frustrated Lewis pair framework. Chemical Communications, 2017, 53, 633-635.	2.2	26
172	Catalytic Difunctionalization of Unactivated Alkenes with Unreactive Hexamethyldisilane through Regeneration of Silylium Ions. Angewandte Chemie - International Edition, 2019, 58, 17307-17311.	7.2	26
173	Fast Quantum Chemical Simulations of Infrared Spectra of Organic Compounds with the B97-3c Composite Method. Journal of Physical Chemistry A, 2019, 123, 3802-3808.	1.1	26
174	Selective Catalytic Frustrated Lewis Pair Hydrogenation of CO₂ in the Presence of Silylhalides. Angewandte Chemie - International Edition, 2021, 60, 25771-25775.	7.2	26
175	Boron Lewis Acid-Catalyzed Regioselective Hydrothiolation of Conjugated Dienes with Thiols. ACS Catalysis, 2019, 9, 11627-11633.	5.5	25
176	Folding of unstructured peptoids and formation of hetero-bimetallic peptoid complexes upon side-chain-to-metal coordination. Chemical Science, 2019, 10, 620-632.	3.7	25
177	TEMPO-Mediated Catalysis of the Sterically Hindered Hydrogen Atom Transfer Reaction between (C₅Ph₅)Cr(CO)₃H and a Trityl Radical. Journal of the American Chemical Society, 2019, 141, 1882-1886.	6.6	25
178	Nonlinear-response properties in a simplified time-dependent density functional theory (sTD-DFT) framework: Evaluation of excited-state absorption spectra. Journal of Chemical Physics, 2019, 150, 094112.	1.2	25
179	Simplified time-dependent density functional theory (sTD-DFT) for molecular optical rotation. Journal of Chemical Physics, 2020, 153, 084116.	1.2	25
180	Quantification of Noncovalent Interactions in Azideâ€“Pnictogen, â€“Chalcogen, and â€“Halogen Contacts. Chemistry - A European Journal, 2021, 27, 4627-4639.	1.7	25

#	Article	IF	Citations
181	The Association of Two â€œFrustratedâ€•Lewis Pairs by Stateâ€•ofâ€•theâ€•Art Quantum Chemical Methods. Israel Journal of Chemistry, 2015, 55, 235-242.	1.0	23
182	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.	1.1	23
183	Exhaustively Trichlorosilylated C₁ and C₂ Building Blocks: Beyond the MÃ¼llerâ€“Rochow Direct Process. Journal of the American Chemical Society, 2018, 140, 9696-9708.	6.6	23
184	PCM-ROKS for the Description of Charge-Transfer States in Solution: Singletâ€“Triplet Gaps with Chemical Accuracy from Open-Shell Kohnâ€“Sham Reaction-Field Calculations. Journal of Physical Chemistry Letters, 2021, 12, 8470-8480.	2.1	23
185	A Frustrated Phosphaneâ€“Borane Lewis Pair and Hydrogen: A Kinetics Study. Chemistry - A European Journal, 2016, 22, 11958-11961.	1.7	22
186	Trapping Experiments on a Trichlorosilanide Anion: a Key Intermediate of Halogenosilane Chemistry. Inorganic Chemistry, 2017, 56, 8683-8688.	1.9	22
187	Pulsed EPR Dipolar Spectroscopy on Spin Pairs with one Highly Anisotropic Spin Center: The Lowâ€•Spin Fe^{III} Case. Chemistry - A European Journal, 2019, 25, 14388-14398.	1.7	22
188	Modeling Transition Metal Reactions with Range-Separated Functionals. Journal of Chemical Theory and Computation, 2013, 9, 2286-2299.	2.3	21
189	Isolation and Computational Studies of a Series of Terphenyl Substituted Diplumbynes with Ligand Dependent Leadâ€“Lead Multiple-Bonding Character. Journal of the American Chemical Society, 2019, 141, 14370-14383.	6.6	21
190	Structure Optimisation of Large Transitionâ€•Metal Complexes with Extended Tightâ€•Binding Methods. Angewandte Chemie, 2019, 131, 11195-11204.	1.6	21
191	A Frustrated and Confused Lewis Pair. Angewandte Chemie - International Edition, 2016, 55, 14335-14339.	7.2	20
192	Quantum Chemical Dissection of the Shortest P=Oâ‹…â‹…â‹…I Halogen Bond: The Decisive Role of Crystal Packing Effects. Chemistry - A European Journal, 2017, 23, 5687-5691.	1.7	20
193	The Chiral Trimer and a Metastable Chiral Dimer of Achiral Hexafluoroisopropanol: A Multiâ€•Messenger Study. Angewandte Chemie, 2019, 131, 5134-5138.	1.6	20
194	Oxidation Under Reductive Conditions: From Benzylic Ethers to Acetals with Perfect Atomâ€•Economy by Titanocene(III) Catalysis. Angewandte Chemie - International Edition, 2021, 60, 5482-5488.	7.2	20
195	[Cl@Si₂₀H₂₀]^{â^’}: Parent Siladodecahedrane with Endohedral Chloride Ion. Journal of the American Chemical Society, 2021, 143, 10865-10871.	6.6	20
196	Ein achtkerniger metallosupramolekularer WÃ¼rfel mit Spinâ€•Crossoverâ€•Eigenschaften. Angewandte Chemie, 2017, 129, 5012-5017.	1.6	19
197	Donorâ€“acceptor interactions between cyclic trinuclear pyridinate gold(<scp>i</scp>)-complexes and electron-poor guests: nature and energetics of guest-binding and templating on graphite. Chemical Science, 2018, 9, 3477-3483.	3.7	19
198	Synthesis of 1,3â€•Amino Alcohols by Hydroxyâ€•Directed Aziridination and Aziridine Hydrosilylation. Angewandte Chemie - International Edition, 2018, 57, 13528-13532.	7.2	19

#	Article	IF	Citations
199	A dispersion-corrected density functional theory case study on ethyl acetate conformers, dimer, and molecular crystal. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	18
200	A Case Study of Mechanical Strain in Supramolecular Complexes to Manipulate the Spin State of Iron(II) Centres. European Journal of Inorganic Chemistry, 2015, 2015, 5503-5510.	1.0	18
201	Diastereoselective Selfâ€Assembly of a Neutral Dinuclear Doubleâ€Stranded Zinc(II) Helicate via Narcissistic Selfâ€Sorting. Chemistry - A European Journal, 2017, 23, 12380-12386.	1.7	18
202	Heterobifunctional Rotaxanes for Asymmetric Catalysis. Angewandte Chemie, 2020, 132, 5140-5145.	1.6	18
203	Fast and Accurate Quantum Chemical Modeling of Infrared Spectra of Condensed-Phase Systems. Journal of Physical Chemistry B, 2020, 124, 6664-6670.	1.2	18
204	Efficient Quantum-Chemical Calculations of Acid Dissociation Constants from Free-Energy Relationships. Journal of Physical Chemistry A, 2021, 125, 5681-5692.	1.1	18
205	Reactions of a Dilithiomethane with CO and N₂O: An Avenue to an Anionic Ketene and a Hexafunctionalized Benzene. Angewandte Chemie - International Edition, 2021, 60, 25281-25285.	7.2	18
206	Automated Quantum Chemistry-Based Calculation of Optical Rotation for Large Flexible Molecules. Journal of Organic Chemistry, 2021, 86, 15522-15531.	1.7	18
207	Quantum Chemical Calculation and Evaluation of Partition Coefficients for Classical and Emerging Environmentally Relevant Organic Compounds. Environmental Science & Technology, 2022, 56, 379-391.	4.6	18
208	Accurate Thermochemistry for Large Molecules with Modern Density Functionals. Topics in Current Chemistry, 2014, , 1-23.	4.0	17
209	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.	1.1	17
210	Designing a Solution-Stable Distannene: The Decisive Role of London Dispersion Effects in the Structure and Properties of {Sn(C₆H₂-2,4,6-Cy₃)₂}₂ (Cy = Cyclohexyl). Journal of the American Chemical Society, 2021, 143, 21478-21483.	6.6	17
211	Synthesis and Rearrangement of Pâ€Nitroxylâ€Substituted P^{III} and P^V Phosphanes: A Combined Experimental and Theoretical Case Study. Chemistry - A European Journal, 2016, 22, 10102-10110.	1.7	16
212	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.	0.6	16
213	Pulsed EPR Dipolar Spectroscopy under the Breakdown of the Highâ€Field Approximation: The Highâ€Spin Iron(III) Case. Chemistry - A European Journal, 2019, 25, 8820-8828.	1.7	16
214	Reduction of Phosphine Oxide by Using Chlorination Reagents and Dihydrogen: DFT Mechanistic Insights. Chemistry - A European Journal, 2019, 25, 4670-4672.	1.7	16
215	Revisiting conformations of methyl lactate in water and methanol. Journal of Chemical Physics, 2021, 155, 024507.	1.2	16
216	Conformational Energy Benchmark for Longer n-Alkane Chains. Journal of Physical Chemistry A, 2022, 126, 3521-3535.	1.1	16

#	Article	IF	Citations
217	Perspective on Simplified Quantum Chemistry Methods for Excited States and Response Properties. Journal of Physical Chemistry A, 2021, 125, 3841-3851.	1.1	15
218	Facile Synthesis of Cyanide and Isocyanides from CO. Angewandte Chemie - International Edition, 2021, 60, 16965-16969.	7.2	15
219	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.	1.2	15
220	Towards understanding solvation effects on the conformational entropy of non-rigid molecules. Physical Chemistry Chemical Physics, 2022, 24, 12249-12259.	1.3	15
221	The Role of Packing, Dispersion, Electrostatics, and Solvation in Highâ€Affinity Complexes of Cucurbit[n]urils with Uncharged Polar Guests. Chemistry - A European Journal, 2022, 28, .	1.7	15
222	Strong Evidence of a Phosphanoxyl Complex: Formation, Bonding, and Reactivity of Ligated Phosphorus Analogues of Nitroxides. Angewandte Chemie - International Edition, 2016, 55, 14439-14443.	7.2	14
223	Frustrated Lewis Pair Catalyzed Reduction of Carbon Dioxide Using Hydroboranes: New DFT Mechanistic Insights. ChemCatChem, 2020, 12, 3656-3660.	1.8	14
224	Comprehensive Benchmark Study on the Calculation of ²⁹Si NMR Chemical Shifts. Inorganic Chemistry, 2021, 60, 272-285.	1.9	14
225	Titanoceneâ€Catalyzed [2+2] Cycloaddition of Bisenones and Comparison with Photoredox Catalysis and Established Methods. Angewandte Chemie - International Edition, 2021, 60, 14339-14344.	7.2	14
226	Cyclic Amine/Borane Lewis Pairs by the Reaction of N,Nâ€Diallylaniline with Lancasterâ€²s H₂Bâ€C₆F₅ Reagent. Chemistry - an Asian Journal, 2016, 11, 1394-1399.	1.7	13
227	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.	1.7	13
228	Unimolecular decomposition pathways of negatively charged nitriles by ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2016, 18, 31017-31026.	1.3	13
229	Dynamic Structural Effects on the Second-Harmonic Generation of Tryptophane-Rich Peptides and Gramicidin A. Journal of Physical Chemistry B, 2020, 124, 2568-2578.	1.2	13
230	Boron-Catalyzed Hydroarylation of 1,3-Dienes with Arylamines. Organic Letters, 2021, 23, 8952-8957.	2.4	13
231	Increased Antiaromaticity through Pentalene Connection in [n]Cyclo-1,5-dibenzopentalenes. Organic Letters, 2022, 24, 983-988.	2.4	13
232	Towards Reagents for Bimetallic Activation Reactions: Polyhydride Complexes with Ru2H3, Ru2ZnH6, and Cu2Ru2H6Cores. European Journal of Inorganic Chemistry, 2013, 2013, 3039-3048.	1.0	12
233	Influencing the Selfâ€Sorting Behavior of [2.2]Paracyclophaneâ€Based Ligands by Introducing Isostructural Binding Motifs. Chemistry - A European Journal, 2020, 26, 3335-3347.	1.7	12
234	Calculation of improved enthalpy and entropy of vaporization by a modified partition function in quantum cluster equilibrium theory. Journal of Chemical Physics, 2021, 155, 104101.	1.2	12

#	Article	IF	Citations
235	Efficient structural and energetic screening of fullerene encapsulation in a large supramolecular double decker macrocycle. Journal of the Serbian Chemical Society, 2019, 84, 837-844.	0.4	12
236	Computerâ€aided simulation of infrared spectra of ethanol conformations in gas, liquid and in <scp>CCl₄</scp> solution. Journal of Computational Chemistry, 2022, 43, 279-288.	1.5	12
237	Intermolecular Carbosilylation of Î±â€Olefins with C(sp3)â€“C(sp) Bond Formation Involving Silyliumâ€Ion Regeneration. Angewandte Chemie - International Edition, 2022, , .	7.2	12
238	Benzimidazolylquinoxalines: novel fluorophores with tuneable sensitivity to solvent effects. Physical Chemistry Chemical Physics, 2017, 19, 6095-6104.	1.3	11
239	A Unified Strategy for the Chemically Intuitive Interpretation of Molecular Optical Response Properties. Journal of Chemical Theory and Computation, 2020, 16, 7709-7720.	2.3	11
240	Mechanistic Insights for Nitromethane Activation into Reactive Nitrogenating Reagents. ChemCatChem, 2021, 13, 2132-2137.	1.8	11
241	Frustrated Lewis pair catalyzed hydrodehalogenation of benzyl-halides. Chemical Communications, 2022, 58, 1175-1178.	2.2	11
242	Benchmark Study on the Calculation of ¹¹⁹Sn NMR Chemical Shifts. Inorganic Chemistry, 2022, 61, 3903-3917.	1.9	11
243	Synthesis of Î¼₂â€Oxoâ€Bridged Iron(III) Tetraphenylporphyrinâ€“Spacerâ€“Nitroxide Dimers and their Structural and Dynamics Characterization by using EPR and MD Simulations. Chemistry - A European Journal, 2019, 25, 2586-2596.	1.7	10
244	Boraneâ€Catalyzed Hydrogenation of Tertiary Amides Activated by Oxalyl Chloride: DFT Mechanistic Insights. European Journal of Organic Chemistry, 2019, 2019, 4609-4612.	1.2	10
245	Oxidation Under Reductive Conditions: From Benzylic Ethers to Acetals with Perfect Atomâ€Economy by Titanocene(III) Catalysis. Angewandte Chemie, 2021, 133, 5542-5548.	1.6	10
246	Hydrocarbon Macrocycle Conformer Ensembles and ¹³Câ€NMR Spectra. Angewandte Chemie - International Edition, 2022, 61, .	7.2	10
247	Synthesis, Chiral Resolution, and Absolute Configuration of Functionalized TrÃ¶gerâ€™s Base Derivatives: Part III. Synthesis, 2015, 47, 3118-3132.	1.2	9
248	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.	0.6	9
249	Mechanistic Insights for Dimethyl Sulfoxide Catalyzed Aromatic Chlorination Reactions. ChemCatChem, 2021, 13, 207-211.	1.8	9
250	Chiral Dibenzopentaleneâ€Based Conjugated Nanohoops through Stereoselective Synthesis. Angewandte Chemie, 2021, 133, 10775-10784.	1.6	9
251	LiAlH 4 â€catalyzed Imine Hydrogenation with Dihydrogen: New DFT Mechanistic Insights. ChemCatChem, 2021, 13, 3401-3404.	1.8	9
252	Hydrogenation of Secondary Amides using Phosphane Oxide and Frustrated Lewis Pair Catalysis. Chemistry - A European Journal, 2021, 27, 14179-14183.	1.7	9

#	Article	IF	Citations
253	The State of Fortran. Computing in Science and Engineering, 2022, 24, 63-72.	1.2	9
254	A multi-scale approach to characterize pure CH4, CF4, and CH4/CF4 mixtures. Journal of Chemical Physics, 2015, 142, 164508.	1.2	8
255	Indirect synthesis of a pair of formal methane activation products at a phosphane/borane frustrated Lewis pair. Dalton Transactions, 2016, 45, 19230-19233.	1.6	8
256	On the hydrogen activation by frustrated Lewis pairs in the solid state: benchmark studies and theoretical insights. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2017, 375, 20170006.	1.6	8
257	Cooperative Organocatalysis: A Systematic Investigation of Covalently Linked Organophosphoric Acids for the Stereoselective Transfer Hydrogenation of Quinolines. European Journal of Organic Chemistry, 2019, 2019, 5190-5195.	1.2	8
258	Comment on â€œThe Nature of Chalcogenâ€Bondingâ€Type Telluriumâ€“Nitrogen Interactionsâ€: Fixing the Description of Finiteâ€Temperature Effects Restores the Agreement Between Experiment and Theory. Angewandte Chemie - International Edition, 2021, 60, 13144-13149.	7.2	8
259	Nanoscale Ï€-conjugated ladders. Nature Communications, 2021, 12, 6614.	5.8	8
260	Quantum Chemistryâ€based Molecular Dynamics Simulations as a Tool for the Assignment of ESIâ€MS/MS Spectra of Drug Molecules. Chemistry - A European Journal, 2022, 28, .	1.7	8
261	Optimization of the r²SCAN-3c Composite Electronic-Structure Method for Use with Slater-Type Orbital Basis Sets. Journal of Physical Chemistry A, 2022, 126, 3826-3838.	1.1	8
262	Predicting the Mass Spectra of Environmental Pollutants Using Computational Chemistry: A Case Study and Critical Evaluation. Journal of the American Society for Mass Spectrometry, 2021, 32, 1508-1518.	1.2	7
263	Steric Influence on Reactions of Benzyl Potassium Species with CO. Chemistry - an Asian Journal, 2021, 16, 3640-3644.	1.7	7
264	Building up Strain in One Step: Synthesis of an Edgeâ€Fused Double Silacyclobutene from an Extensively Trichlorosilylated Butadiene Dianion. Angewandte Chemie - International Edition, 2020, 59, 16181-16187.	7.2	6
265	A Primary Acyl Phosphine Stabilized by a Phosphonium Ylide. Angewandte Chemie - International Edition, 2021, 60, 18547-18551.	7.2	6
266	Ligand Protonation at Carbon, not Nitrogen, during H₂ Production with Amine-Rich Iron Electrocatalysts. Inorganic Chemistry, 2021, 60, 17407-17413.	1.9	6
267	Itâ€™s Complicated: On Relativistic Effects and Periodic Trends in the Melting and Boiling Points of the Group 11 Coinage Metals. Journal of the American Chemical Society, 2022, 144, 485-494.	6.6	6
268	Are Fully Conjugated Expanded Indenofluorenes Analogues and Diindeno[n]thiophene Derivatives Diradicals? A Simplified (Spin-Flip) Time-Dependent Density Functional Theory [(SF-)sTD-DFT] Study. Journal of Physical Chemistry A, 2019, 123, 9828-9839.	1.1	5
269	Mechanistic Insights for Anilineâ€Catalyzed Halogenation Reactions. ChemCatChem, 2020, 12, 5369-5373.	1.8	5
270	Mechanistic Insights for Iodane Mediated Aromatic Halogenation Reactions. ChemCatChem, 2020, 12, 6186-6190.	1.8	5

#	Article	IF	Citations
271	Mechanistic Insights for Acidâ€catalyzed Rearrangement of Quinoxalinâ€2â€one with Diamine and Enamine. ChemCatChem, 2021, 13, 1503-1508.	1.8	5
272	Reactions of a Dilithiomethane with CO and N₂O: An Avenue to an Anionic Ketene and a Hexafunctionalized Benzene. Angewandte Chemie, 2021, 133, 25485-25489.	1.6	5
273	All-Atom Quantum Mechanical Calculation of the Second-Harmonic Generation of Fluorescent Proteins. Journal of Physical Chemistry Letters, 2021, 12, 9684-9690.	2.1	5
274	Hydrogen atom transfer rates from Tp-containing metal-hydrides to trityl radicals. Canadian Journal of Chemistry, 2021, 99, 216-220.	0.6	5
275	The Varied Frustrated Lewis Pair Reactivity of the Germylene Phosphaketene (CH{(CMe)(2,6â€ⁱPr₂C₆H₃N)}₂)GePCO. Chemistry - A European Journal, 2022, 28, .	1.7	5
276	Substitution effect and effect of axleâ€™s flexibility at (pseudo-)rotaxanes. Beilstein Journal of Organic Chemistry, 2014, 10, 1299-1307.	1.3	4
277	Synthesis of 1,3â€Amino Alcohols by Hydroxyâ€Directed Aziridination and Aziridine Hydrosilylation. Angewandte Chemie, 2018, 130, 13716-13720.	1.6	4
278	Extension of the element parameter set for ultra-fast excitation spectra calculation (sTDA-xTB). Molecular Physics, 2019, 117, 1104-1116.	0.8	4
279	The power of trichlorosilylation: isolable trisilylated allyl anions, allyl radicals, and allenyl anions. Chemical Science, 2021, 12, 12419-12428.	3.7	4
280	Comment on â€œThe Nature of Chalcogenâ€Bondingâ€Type Telluriumâ€“Nitrogen Interactionsâ€: Fixing the Description of Finiteâ€Temperature Effects Restores the Agreement Between Experiment and Theory. Angewandte Chemie, 2021, 133, 13252-13257.	1.6	4
281	Titanoceneâ€Catalyzed [2+2] Cycloaddition of Bisenones and Comparison with Photoredox Catalysis and Established Methods. Angewandte Chemie, 2021, 133, 14460-14465.	1.6	4
282	High-Throughput Non-targeted Chemical Structure Identification Using Gas-Phase Infrared Spectra. Analytical Chemistry, 2021, 93, 10688-10696.	3.2	4
283	Supramolecular Nanopatterns of Molecular Spoked Wheels with Orthogonal Pillars: The Observation of a Fullerene Haze. Angewandte Chemie - International Edition, 2021, 60, 27264-27270.	7.2	4
284	The Nonâ€Ancillary Nature of Trimethylsilylamide Substituents in Boranes and Borinium Cations. Chemistry - A European Journal, 2022, 28, .	1.7	4
285	Quickstart guide to model structures and interactions of artificial molecular muscles with efficient computational methods. Chemical Communications, 2021, 58, 258-261.	2.2	3
286	Design, Synthesis, EPRâ€Studies and Conformational Bias of Novel Spinâ€Labeled DCCâ€Analogues for the Highly Regioselective Labeling of Aliphatic and Aromatic Carboxylic Acids. Chemistry - A European Journal, 2016, 22, 9591-9598.	1.7	2
287	Structural and Conformational Studies on Carboxamides of 5,6-Diaminouracilsâ€”Precursors of Biologically Active Xanthine Derivatives. Molecules, 2019, 24, 2168.	1.7	2
288	Building up Strain in One Step: Synthesis of an Edgeâ€Fused Double Silacyclobutene from an Extensively Trichlorosilylated Butadiene Dianion. Angewandte Chemie, 2020, 132, 16315-16321.	1.6	2

#	Article	IF	Citations
289	Frustrated Lewisâ€Pair Neighbors at the Xanthene Framework: Epimerization at Phosphorus and Cooperative Formation of Macrocyclic Adduct Structures. Chemistry - A European Journal, 2021, 27, 12104-12114.	1.7	2
290	Stereochemical Behavior of Pairs of Pâ€stereogenic Phosphanyl Groups at the Dimethylxanthene Backbone. Chemistry - A European Journal, 2022, , .	1.7	2
291	Câ€H Deprotonation and C=C Hydrogenation of Nâ€heterocyclic Olefin with Calcium Hydride Complexes: Cooperative Caâ€Hâ€Ca Bridge versus Terminal Caâ€H bond. ChemCatChem, 0, , .	1.8	2
292	Frontispiece: An Octanuclear Metallosupramolecular Cage Designed To Exhibit Spinâ€Crossover Behavior. Angewandte Chemie - International Edition, 2017, 56, .	7.2	1
293	Sensory Perception of Nonâ€Deuterated and Deuterated Organic Compounds. Chemistry - A European Journal, 2021, 27, 1046-1056.	1.7	1
294	A Primary Acyl Phosphine Stabilized by a Phosphonium Ylide. Angewandte Chemie, 2021, 133, 18695-18699.	1.6	1
295	Hydrocarbon Macrocycle Conformer Ensembles and 13Câ€NMR spectra. Angewandte Chemie, 0, , .	1.6	1
296	The long-awaited synthesis and self-assembly of a small rigid C₃-symmetric trilactam. Chemical Communications, 2022, 58, 3751-3754.	2.2	1
297	Computational study of groundâ€state properties of Î¼ ₂ â€bridged group 14 porphyrinic sandwich complexes. Journal of Computational Chemistry, 2022, , .	1.5	1
298	RÃ¼cktitelbild: Functional Mechanically Interlocked Molecules: Asymmetric Organocatalysis with a Catenated Bifunctional BrÃ¸nsted Acid (Angew. Chem. 38/2017). Angewandte Chemie, 2017, 129, 11814-11814.	1.6	0
299	Frontispiz: Ein achtkerniger metallosupramolekularer WÃ¼rfel mit Spinâ€Crossoverâ€Eigenschaften. Angewandte Chemie, 2017, 129, .	1.6	0
300	RÃ¼cktitelbild: Heterobifunctional Rotaxanes for Asymmetric Catalysis (Angew. Chem. 13/2020). Angewandte Chemie, 2020, 132, 5446-5446.	1.6	0