Stefan Grimme

List of Publications by Year
in descending order

357 papers	128,975 citations	2322 98 h-index	102 350 g-index
375 all docs	375 docs citations	375 times ranked	68001 citing authors

#	Article	IF	Citations
1	A consistent and accurate<i>ab initio</i>parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. Journal of Chemical Physics, 2010, 132, 154104.	3.0	35,972
2	Semiempirical GGA-type density functional constructed with a long-range dispersion correction. Journal of Computational Chemistry, 2006, 27, 1787-1799.	3.3	24,222
3	Effect of the damping function in dispersion corrected density functional theory. Journal of Computational Chemistry, 2011, 32, 1456-1465.	3.3	15,980
4	Accurate description of van der Waals complexes by density functional theory including empirical corrections. Journal of Computational Chemistry, 2004, 25, 1463-1473.	3.3	4,372
5	Semiempirical hybrid density functional with perturbative second-order correlation. Journal of Chemical Physics, 2006, 124, 034108.	3.0	2,729
6	Density functional theory with London dispersion corrections. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 211-228.	14.6	2,030
7	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
8	A thorough benchmark of density functional methods for general main group thermochemistry, kinetics, and noncovalent interactions. Physical Chemistry Chemical Physics, 2011, 13, 6670.	2.8	1,627
9	Improved second-order MÃ¸llerâ€"Plesset perturbation theory by separate scaling of parallel- and antiparallel-spin pair correlation energies. Journal of Chemical Physics, 2003, 118, 9095-9102.	3.0	1,607
10	Supramolecular Binding Thermodynamics by Dispersionâ€Corrected Density Functional Theory. Chemistry - A European Journal, 2012, 18, 9955-9964.	3.3	1,346
11	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.	2.8	1,230
12	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 (<i>Z</i> = 1â€"86). Journal of Chemical Theory and Computation, 2017, 13, 1989-2009.	5.3	1,072
13	Efficient and Accurate Double-Hybrid-Meta-GGA Density Functionalsâ€"Evaluation with the Extended GMTKN30 Database for General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions. Journal of Chemical Theory and Computation, 2011, 7, 291-309.	5.3	1,035
14	Dispersion-Corrected Mean-Field Electronic Structure Methods. Chemical Reviews, 2016, 116, 5105-5154.	47.7	1,032
15	Double-hybrid density functionals with long-range dispersion corrections: higher accuracy and extended applicability. Physical Chemistry Chemical Physics, 2007, 9, 3397.	2.8	979
16	Automated exploration of the low-energy chemical space with fast quantum chemical methods. Physical Chemistry Chemical Physics, 2020, 22, 7169-7192.	2.8	966
17	Do Special Noncovalent Ï€â€"Ï€ Stacking Interactions Really Exist?. Angewandte Chemie - International Edition, 2008, 47, 3430-3434.	13.8	928
18	A generally applicable atomic-charge dependent London dispersion correction. Journal of Chemical Physics, 2019, 150, 154122.	3.0	697

#	Article	IF	Citations
19	Density functional theory with dispersion corrections for supramolecular structures, aggregates, and complexes of (bio)organic molecules. Organic and Biomolecular Chemistry, 2007, 5, 741-758.	2.8	683
20	Reversible Metalâ€Free Carbon Dioxide Binding by Frustrated Lewis Pairs. Angewandte Chemie - International Edition, 2009, 48, 6643-6646.	13.8	680
21	A combination of Kohnâ€“Sham density functional theory and multi-reference configuration interaction methods. Journal of Chemical Physics, 1999, 111, 5645-5655.	3.0	635
22	Extension of the D3 dispersion coefficient model. Journal of Chemical Physics, 2017, 147, 034112.	3.0	617
23	Consistent structures and interactions by density functional theory with small atomic orbital basis sets. Journal of Chemical Physics, 2015, 143, 054107.	3.0	605
24	Extended <scp>tightâ€binding</scp> quantum chemistry methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1493.	14.6	596
25	Rapid intramolecular heterolytic dihydrogen activation by a four-membered heterocyclic phosphaneâ€“borane adduct. Chemical Communications, 2007, , 5072.	4.1	563
26	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.	3.0	556
27	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.	5.3	551
28	Towards chemical accuracy for the thermodynamics of large molecules: new hybrid density functionals including non-local correlation effects. Physical Chemistry Chemical Physics, 2006, 8, 4398.	2.8	538
29	DFT-D3 Study of Some Molecular Crystals. Journal of Physical Chemistry C, 2014, 118, 7615-7621.	3.1	457
30	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.	1.1	445
31	Why the Standard B3LYP/6-31G* Model Chemistry Should Not Be Used in DFT Calculations of Molecular Thermochemistry: Understanding and Correcting the Problem. Journal of Organic Chemistry, 2012, 77, 10824-10834.	3.2	407
32	Double-hybrid density functional theory for excited electronic states of molecules. Journal of Chemical Physics, 2007, 127, 154116.	3.0	404
33	B97-3c: A revised low-cost variant of the B97-D density functional method. Journal of Chemical Physics, 2018, 148, 064104.	3.0	400
34	The Mechanism of Dihydrogen Activation by Frustrated Lewis Pairs Revisited. Angewandte Chemie - International Edition, 2010, 49, 1402-1405.	13.8	394
35	A General Database for Main Group Thermochemistry, Kinetics, and Noncovalent Interactions âˆ’ Assessment of Common and Reparameterized (<i>meta</i>-)GGA Density Functionals. Journal of Chemical Theory and Computation, 2010, 6, 107-126.	5.3	389
36	Benchmarking of London Dispersion-Accounting Density Functional Theory Methods on Very Large Molecular Complexes. Journal of Chemical Theory and Computation, 2013, 9, 1580-1591.	5.3	362

#	Article	IF	Citations
37	Seemingly Simple Stereoelectronic Effects in Alkane Isomers and the Implications for Kohnâ€“Sham Density Functional Theory. Angewandte Chemie - International Edition, 2006, 45, 4460-4464.	13.8	360
38	Corrected small basis set Hartreeâ€Fock method for large systems. Journal of Computational Chemistry, 2013, 34, 1672-1685.	3.3	358
39	Theoretical Thermodynamics for Large Molecules: Walking the Thin Line between Accuracy and Computational Cost. Accounts of Chemical Research, 2008, 41, 569-579.	15.6	329
40	Systemâ€Dependent Dispersion Coefficients for the DFTâ€D3 Treatment of Adsorption Processes on Ionic Surfaces. ChemPhysChem, 2011, 12, 3414-3420.	2.1	318
41	Doubleâ€hybrid density functionals. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 576-600.	14.6	292
42	r2SCAN-3c: A â€œSwiss army knifeâ€• composite electronic-structure method. Journal of Chemical Physics, 2021, 154, 064103.	3.0	290
43	Benchmarking Density Functional Methods against the S66 and S66x8 Datasets for Nonâ€Covalent Interactions. ChemPhysChem, 2011, 12, 3421-3433.	2.1	283
44	Full Selectivity Control in Cobalt(III)â€Catalyzed Câˆ’H Alkylations by Switching of the Câˆ’H Activation Mechanism. Angewandte Chemie - International Edition, 2017, 56, 10378-10382.	13.8	243
45	A simplified Tamm-Dancoff density functional approach for the electronic excitation spectra of very large molecules. Journal of Chemical Physics, 2013, 138, 244104.	3.0	242
46	Accurate Calculation of the Heats of Formation for Large Main Group Compounds with Spin-Component Scaled MP2 Methods. Journal of Physical Chemistry A, 2005, 109, 3067-3077.	2.5	241
47	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.	2.8	238
48	How to Compute Isomerization Energies of Organic Molecules with Quantum Chemical Methods. Journal of Organic Chemistry, 2007, 72, 2118-2126.	3.2	234
49	Steric Crowding Can Stabilize a Labile Molecule: Solving the Hexaphenylethane Riddle. Angewandte Chemie - International Edition, 2011, 50, 12639-12642.	13.8	232
50	Metalâ€free Catalytic Olefin Hydrogenation: Lowâ€Temperature H₂â€…Activation by Frustrated Lewis Pairs. Angewandte Chemie - International Edition, 2012, 51, 10164-10168.	13.8	230
51	Robust Atomistic Modeling of Materials, Organometallic, and Biochemical Systems. Angewandte Chemie - International Edition, 2020, 59, 15665-15673.	13.8	224
52	Reactions of an Intramolecular Frustrated Lewis Pair with Unsaturated Substrates: Evidence for a Concerted Olefin Addition Reaction. Journal of the American Chemical Society, 2009, 131, 12280-12289.	13.7	218
53	â€œMindlessâ€• DFT Benchmarking. Journal of Chemical Theory and Computation, 2009, 5, 993-1003.	5.3	215
54	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.	5.3	213

#	Article	IF	Citations
55	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
56	Performance of dispersion-corrected density functional theory for the interactions in ionic liquids. Physical Chemistry Chemical Physics, 2012, 14, 4875.	2.8	202
57	Comprehensive Thermochemical Benchmark Set of Realistic Closed-Shell Metal Organic Reactions. Journal of Chemical Theory and Computation, 2018, 14, 2596-2608.	5.3	202
58	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.	5.3	199
59	Spinâ€componentâ€scaled electron correlation methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 886-906.	14.6	197
60	A Practicable Realâ€Space Measure and Visualization of Static Electronâ€Correlation Effects. Angewandte Chemie - International Edition, 2015, 54, 12308-12313.	13.8	194
61	An improved method for density functional calculations of the frequency-dependent optical rotation. Chemical Physics Letters, 2002, 361, 321-328.	2.6	189
62	On the Importance of the Dispersion Energy for the Thermodynamic Stability of Molecules. ChemPhysChem, 2011, 12, 1258-1261.	2.1	188
63	Comprehensive Benchmark of Association (Free) Energies of Realistic Hostâ€"Guest Complexes. Journal of Chemical Theory and Computation, 2015, 11, 3785-3801.	5.3	188
64	Robust and Efficient Implicit Solvation Model for Fast Semiempirical Methods. Journal of Chemical Theory and Computation, 2021, 17, 4250-4261.	5.3	186
65	Capture of NO by a Frustrated Lewis Pair: A New Type of Persistent <i>N</i>â€Oxyl Radical. Angewandte Chemie - International Edition, 2011, 50, 7567-7571.	13.8	181
66	Combinations of Ethers and B(C₆F₅)₃ Function as Hydrogenation Catalysts. Angewandte Chemie - International Edition, 2013, 52, 7492-7495.	13.8	180
67	Reaction of Frustrated Lewis Pairs with Conjugated Ynonesâ€Selective Hydrogenation of the Carbonâ€"Carbon Triple Bond. Angewandte Chemie - International Edition, 2011, 50, 7183-7186.	13.8	169
68	Câ€"F/Câ€"H Functionalization by Manganese(I) Catalysis: Expedient (Per)Fluoro-Allylations and Alkenylations. ACS Catalysis, 2017, 7, 4209-4213.	11.2	165
69	Is Spin-Component Scaled Second-Order MÃ¸llerâ€"Plesset Perturbation Theory an Appropriate Method for the Study of Noncovalent Interactions in Molecules?. Journal of Physical Chemistry A, 2007, 111, 4862-4868.	2.5	164
70	On the Importance of Electron Correlation Effects for theÏ€-Ï€ Interactions in Cyclophanes. Chemistry - A European Journal, 2004, 10, 3423-3429.	3.3	162
71	Calculation of frequency dependent optical rotation using density functional response theory. Chemical Physics Letters, 2001, 339, 380-388.	2.6	158
72	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

#	Article	IF	Citations
73	Accurate Modeling of Organic Molecular Crystals by Dispersion-Corrected Density Functional Tight Binding (DFTB). Journal of Physical Chemistry Letters, 2014, 5, 1785-1789.	4.6	155
74	A General Quantum Mechanically Derived Force Field (QMDFF) for Molecules and Condensed Phase Simulations. Journal of Chemical Theory and Computation, 2014, 10, 4497-4514.	5.3	154
75	<i>N</i>,<i>N</i>-Addition of Frustrated Lewis Pairs to Nitric Oxide: An Easy Entry to a Unique Family of Aminoxyl Radicals. Journal of the American Chemical Society, 2012, 134, 10156-10168.	13.7	153
76	Reactions of phosphorus/boron frustrated Lewis pairs with SO₂. Chemical Science, 2013, 4, 213-219.	7.4	150
77	Towards First Principles Calculation of Electron Impact Mass Spectra of Molecules. Angewandte Chemie - International Edition, 2013, 52, 6306-6312.	13.8	148
78	CO₂ and Formate Complexes of Phosphine/Borane Frustrated Lewis Pairs. Chemistry - A European Journal, 2011, 17, 9640-9650.	3.3	146
79	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.	1.9	146
80	Facile Carbon Monoxide Reduction at Intramolecular Frustrated Phosphane/Borane Lewis Pair Templates. Angewandte Chemie - International Edition, 2013, 52, 2243-2246.	13.8	143
81	Computational Chemistry: The Fate of Current Methods and Future Challenges. Angewandte Chemie - International Edition, 2018, 57, 4170-4176.	13.8	138
82	Extension and evaluation of the D4 London-dispersion model for periodic systems. Physical Chemistry Chemical Physics, 2020, 22, 8499-8512.	2.8	138
83	Mechanism of Titanocene-Mediated Epoxide Opening through Homolytic Substitution. Journal of the American Chemical Society, 2007, 129, 1359-1371.	13.7	135
84	Cationâˆ'Cation â€œAttractionâ€: When London Dispersion Attraction Wins over Coulomb Repulsion. Inorganic Chemistry, 2011, 50, 2619-2628.	4.0	127
85	London Dispersion Enables the Shortest Intermolecular Hydrocarbon HÂ·Â·Â·H Contact. Journal of the American Chemical Society, 2017, 139, 7428-7431.	13.7	126
86	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.	13.8	125
87	Using dispersion-corrected density functional theory to understand supramolecular binding thermodynamics. Chemical Communications, 2015, 51, 1764-1774.	4.1	125
88	Effects of London dispersion on the isomerization reactions of large organic molecules: a density functional benchmark study. Physical Chemistry Chemical Physics, 2010, 12, 6940.	2.8	123
89	Geometrical Correction for the Inter- and Intramolecular Basis Set Superposition Error in Periodic Density Functional Theory Calculations. Journal of Physical Chemistry A, 2013, 117, 9282-9292.	2.5	123
90	Improved third-order MÃ¸ller-Plesset perturbation theory. Journal of Computational Chemistry, 2003, 24, 1529-1537.	3.3	117

#	ARTICLE	IF	CITATIONS
91	Understanding and Quantifying London Dispersion Effects in Organometallic Complexes. Accounts of Chemical Research, 2019, 52, 258-266.	15.6	117
92	Importance of London dispersion effects for the packing of molecular crystals: a case study for intramolecular stacking in a bis-thiophene derivative. Physical Chemistry Chemical Physics, 2010, 12, 8500.	2.8	115
93	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
94	A Radical Tandem Reaction with Homolytic Cleavage of a Tiï£¿O Bond. Angewandte Chemie - International Edition, 2003, 42, 3687-3690.	13.8	110
95	Exploring the Limits of Frustrated Lewis Pair Chemistry with Alkynes: Detection of a System that Favors 1,1â€Carboboration over Cooperative 1,2â€P/Bâ€Addition. Chemistry - an Asian Journal, 2010, 5, 2199-2208.	3.3	106
96	Efficient Quantum Chemical Calculation of Structure Ensembles and Free Energies for Nonrigid Molecules. Journal of Physical Chemistry A, 2021, 125, 4039-4054.	2.5	105
97	Calculation of the Electronic Spectra of Large Molecules. Reviews in Computational Chemistry, 2004, , 153-218.	1.5	102
98	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.	3.3	102
99	Enantiomerically Pure [M₆L₁₂] or [M₁₂L₂₄] Polyhedra from Flexible Bis(Pyridine) Ligands. Angewandte Chemie - International Edition, 2014, 53, 1693-1698.	13.8	96
100	Consistent Theoretical Description of 1,3-Dipolar Cycloaddition Reactions. Journal of Physical Chemistry A, 2006, 110, 2583-2586.	2.5	95
101	Full Selectivity Control in Cobalt(III)â€Catalyzed Câ^'H Alkylations by Switching of the Câ^'H Activation Mechanism. Angewandte Chemie, 2017, 129, 10514-10518.	2.0	95
102	Mild Cobalt(III)â€Catalyzed Allylative Câ^'F/Câ^'H Functionalizations at Room Temperature. Chemistry - A European Journal, 2017, 23, 12145-12148.	3.3	95
103	Carbonylation Reactions of Intramolecular Vicinal Frustrated Phosphane/Borane Lewis Pairs. Journal of the American Chemical Society, 2013, 135, 18567-18574.	13.7	94
104	Electronic effects of triarylphosphines in metal-free hydrogen activation: a kinetic and computational study. Chemical Science, 2013, 4, 2788.	7.4	93
105	1,1â€Hydroboration and a Borane Adduct of Diphenyldiazomethane: A Potential Prelude to FLPâ€N₂ Chemistry. Angewandte Chemie - International Edition, 2017, 56, 16588-16592.	13.8	93
106	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.	5.3	91
107	Quantum Chemical Benchmark Study on 46 RNA Backbone Families Using a Dinucleotide Unit. Journal of Chemical Theory and Computation, 2015, 11, 4972-4991.	5.3	90
108	Elucidation of the Mechanism of Titanocene-Mediated Epoxide Opening by a Combined Experimental and Theoretical Approach. Angewandte Chemie - International Edition, 2006, 45, 2041-2044.	13.8	89

#	Article	IF	Citations
109	How to Compute Electron Ionization Mass Spectra from First Principles. Journal of Physical Chemistry A, 2016, 120, 3755-3766.	2.5	88
110	Functional Mechanically Interlocked Molecules: Asymmetric Organocatalysis with a Catenated Bifunctional BrÃ¸nsted Acid. Angewandte Chemie - International Edition, 2017, 56, 11456-11459.	13.8	88
111	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.	13.7	86
112	Benchmarking DFT and semiempirical methods on structures and lattice energies for ten ice polymorphs. Journal of Chemical Physics, 2015, 142, 124104.	3.0	84
113	Calculation of absolute molecular entropies and heat capacities made simple. Chemical Science, 2021, 12, 6551-6568.	7.4	83
114	Remarkable coordination behavior of alkyl isocyanides toward unsaturated vicinal frustrated P/B Lewis pairs. Chemical Science, 2013, 4, 2657.	7.4	81
115	1,1â€Hydroboration and a Borane Adduct of Diphenyldiazomethane: A Potential Prelude to FLPâ€N₂ Chemistry. Angewandte Chemie, 2017, 129, 16815-16819.	2.0	81
116	Low-Cost Quantum Chemical Methods for Noncovalent Interactions. Journal of Physical Chemistry Letters, 2014, 5, 4275-4284.	4.6	80
117	B(C₆F₅)₃â€Catalyzed Transfer of Dihydrogen from One Unsaturated Hydrocarbon to Another. Angewandte Chemie - International Edition, 2015, 54, 12158-12162.	13.8	80
118	An Octanuclear Metallosupramolecular Cage Designed To Exhibit Spinâ€Crossover Behavior. Angewandte Chemie - International Edition, 2017, 56, 4930-4935.	13.8	80
119	Quantum chemical calculation of electron ionization mass spectra for general organic and inorganic molecules. Chemical Science, 2017, 8, 4879-4895.	7.4	79
120	Proteinâ€“Ligand Interaction Energies with Dispersion Corrected Density Functional Theory and High-Level Wave Function Based Methods. Journal of Physical Chemistry A, 2011, 115, 11210-11220.	2.5	78
121	New Insights into Frustrated Lewis Pairs: Structural Investigations of Intramolecular Phosphaneâ€“Borane Adducts by Using Modern Solid-State NMR Techniques and DFT Calculations. Journal of the American Chemical Society, 2012, 134, 4236-4249.	13.7	78
122	Substituent Effects and Supramolecular Interactions of Titanocene(III) Chloride: Implications for Catalysis in Single Electron Steps. Journal of the American Chemical Society, 2014, 136, 1663-1671.	13.7	78
123	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.	3.3	78
124	Comprehensive Study of the Thermochemistry of First-Row Transition Metal Compounds by Spin Component Scaled MP2 and MP3 Methods. Organometallics, 2004, 23, 5581-5592.	2.3	77
125	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
126	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.	2.6	77

#	Article	IF	Citations
127	Excited states using the simplified Tammâ€“Dancoff-Approach for range-separated hybrid density functionals: development and application. Physical Chemistry Chemical Physics, 2014, 16, 14408-14419.	2.8	76
128	Assessing Density Functional Theory for Chemically Relevant Open-Shell Transition Metal Reactions. Journal of Chemical Theory and Computation, 2021, 17, 6134-6151.	5.3	75
129	Structural Importance of Secondary Interactions in Molecules: Origin of Unconventional Conformations of Phosphineâ€“Borane Adducts. Chemistry - A European Journal, 2008, 14, 333-343.	3.3	74
130	Reaction of a Bridged Frustrated Lewis Pair with Nitric Oxide: A Kinetics Study. Journal of the American Chemical Society, 2014, 136, 513-519.	13.7	73
131	Dispersion Corrected Hartreeâ€“Fock and Density Functional Theory for Organic Crystal Structure Prediction. Topics in Current Chemistry, 2013, 345, 1-23.	4.0	72
132	Frustrated Lewis Pairâ€Catalyzed Cycloisomerization of 1,5â€Enynes via a 5â€<i>endo</i>â€dig Cyclization/Protodeborylation Sequence. Angewandte Chemie - International Edition, 2016, 55, 4336-4339.	13.8	72
133	Structure Optimisation of Large Transitionâ€Metal Complexes with Extended Tightâ€Binding Methods. Angewandte Chemie - International Edition, 2019, 58, 11078-11087.	13.8	72
134	Mechanistic Study of the Titanocene(III)â€Catalyzed Radical Arylation of Epoxides. Chemistry - A European Journal, 2015, 21, 280-289.	3.3	71
135	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.	13.7	70
136	Ab initio calculations for the optical rotations of conformationally flexible molecules: A case study on six-, seven-, and eight-membered fluorinated cycloalkanol esters. Chirality, 2002, 14, 793-797.	2.6	69
137	Titanoceneâ€Catalyzed Radical Opening of Nâ€Acylated Aziridines. Angewandte Chemie - International Edition, 2017, 56, 12654-12657.	13.8	67
138	Enantiomerically Pure Trinuclear Helicates via Diastereoselective Self-Assembly and Characterization of Their Redox Chemistry. Journal of the American Chemical Society, 2014, 136, 11830-11838.	13.7	65
139	Frustrated Lewis Pair Modification by 1,1-Carboboration: Disclosure of a Phosphine Oxide Triggered Nitrogen Monoxide Addition to an Intramolecular P/B Frustrated Lewis Pair. Journal of the American Chemical Society, 2014, 136, 9014-9027.	13.7	65
140	BNB-Doped Phenalenyls: Modular Synthesis, Optoelectronic Properties, and One-Electron Reduction. Journal of the American Chemical Society, 2020, 142, 11072-11083.	13.7	63
141	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.	13.7	62
142	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.	2.6	62
143	A Radical Roundabout for an Unprecedented Tandem Reaction Including a Homolytic Substitution with a Titanium-Oxygen Bond. European Journal of Organic Chemistry, 2004, 2004, 2337-2351.	2.4	61
144	Stable Borocyclic Radicals via Frustrated Lewis Pair Hydrogenations. Journal of the American Chemical Society, 2016, 138, 2500-2503.	13.7	61

#	Article	IF	Citations
145	Semiautomated Transition State Localization for Organometallic Complexes with Semiempirical Quantum Chemical Methods. Journal of Chemical Theory and Computation, 2020, 16, 2002-2012.	5.3	60
146	Comprehensive theoretical study of all 1812 C₆₀ isomers. Physical Chemistry Chemical Physics, 2017, 19, 14296-14305.	2.8	58
147	Small Atomic Orbital Basis Set Firstâ€Principles Quantum Chemical Methods for Large Molecular and Periodic Systems: A Critical Analysis of Error Sources. ChemistryOpen, 2016, 5, 94-109.	1.9	57
148	Highly Active Titanocene Catalysts for Epoxide Hydrosilylation: Synthesis, Theory, Kinetics, EPR Spectroscopy. Angewandte Chemie - International Edition, 2016, 55, 7671-7675.	13.8	57
149	Heterobifunctional Rotaxanes for Asymmetric Catalysis. Angewandte Chemie - International Edition, 2020, 59, 5102-5107.	13.8	56
150	A computationally efficient double hybrid density functional based on the random phase approximation. Physical Chemistry Chemical Physics, 2016, 18, 20926-20937.	2.8	55
151	HFIPâ€Assisted Single Câˆ’F Bond Activation of Trifluoromethyl Ketones using Visibleâ€Light Photoredox Catalysis. Angewandte Chemie - International Edition, 2022, 61, .	13.8	54
152	Thermochemical benchmarking of hydrocarbon bond separation reaction energies: Jacob's ladder is not reversed!. Molecular Physics, 2010, 108, 2655-2666.	1.7	53
153	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.	1.1	53
154	A general intermolecular force field based on tight-binding quantum chemical calculations. Journal of Chemical Physics, 2017, 147, 161708.	3.0	53
155	Theoretical study on conformational energies of transition metal complexes. Physical Chemistry Chemical Physics, 2021, 23, 287-299.	2.8	52
156	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.	13.7	50
157	Boraneâ€Catalyzed Synthesis of Quinolines Bearing Tetrasubstituted Stereocenters by Hydride Abstractionâ€Induced Electrocyclization. Chemistry - A European Journal, 2018, 24, 16287-16291.	3.3	50
158	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.	2.9	50
159	Screened exchange hybrid density functional for accurate and efficient structures and interaction energies. Physical Chemistry Chemical Physics, 2016, 18, 15519-15523.	2.8	49
160	Automated and efficient quantum chemical determination and energetic ranking of molecular protonation sites. Journal of Computational Chemistry, 2017, 38, 2618-2631.	3.3	49
161	Efficient Computation of Free Energy Contributions for Association Reactions of Large Molecules. Journal of Physical Chemistry Letters, 2020, 11, 6606-6611.	4.6	49
162	Single-Point Hessian Calculations for Improved Vibrational Frequencies and Rigid-Rotor-Harmonic-Oscillator Thermodynamics. Journal of Chemical Theory and Computation, 2021, 17, 1701-1714.	5.3	49

#	Article	IF	Citations
163	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.	3.3	48
164	The frustrated Lewis pair pathway to methylene phosphonium systems. Chemical Science, 2014, 5, 797-803.	7.4	47
165	Lithium Dicyclohexylamide in Transition-Metal-Free Fischerâ€"Tropsch Chemistry. Journal of the American Chemical Society, 2021, 143, 634-638.	13.7	47
166	Selective Oxidation of an Active Intramolecular Amine/Borane Frustrated Lewis Pair with Dioxygen. Journal of the American Chemical Society, 2016, 138, 4302-4305.	13.7	46
167	Towards full Quantumâ€Mechanicsâ€based Proteinâ€"Ligand Binding Affinities. ChemPhysChem, 2017, 18, 898-905.	2.1	46
168	The Chiral Trimer and a Metastable Chiral Dimer of Achiral Hexafluoroisopropanol: A Multiâ€Messenger Study. Angewandte Chemie - International Edition, 2019, 58, 5080-5084.	13.8	46
169	Benchmark Study of Electrochemical Redox Potentials Calculated with Semiempirical and DFT Methods. Journal of Physical Chemistry A, 2020, 124, 7166-7176.	2.5	45
170	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.	5.3	45
171	The furan microsolvation blind challenge for quantum chemical methods: First steps. Journal of Chemical Physics, 2018, 148, 014301.	3.0	44
172	Unusual mass spectrometric dissociation pathway of protonated isoquinoline-3-carboxamides due to multiple reversible water adduct formation in the gas phase. Journal of the American Society for Mass Spectrometry, 2009, 20, 2034-2048.	2.8	43
173	Bismuth as a versatile cation for luminescence in coordination polymers from BiX₃/4,4â€²-bipy: understanding of photophysics by quantum chemical calculations and structural parallels to lanthanides. Dalton Transactions, 2018, 47, 7669-7681.	3.3	43
174	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.	13.7	43
175	Comment on: â€œOn the Accuracy of DFT Methods in Reproducing Ligand Substitution Energies for Transition Metal Complexes in Solution: The Role of Dispersive Interactionsâ€•by H. Jacobsen and L. Cavallo. ChemPhysChem, 2012, 13, 1407-1409.	2.1	42
176	The â€œCatalytic Nitrosyl Effectâ€• NO Bending Boosting the Efficiency of Rhenium Based Alkene Hydrogenations. Journal of the American Chemical Society, 2013, 135, 4088-4102.	13.7	41
177	Fast and Reasonable Geometry Optimization of Lanthanoid Complexes with an Extended Tight Binding Quantum Chemical Method. Inorganic Chemistry, 2017, 56, 12485-12491.	4.0	41
178	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.	3.0	41
179	Robust Atomistic Modeling of Materials, Organometallic, and Biochemical Systems. Angewandte Chemie, 2020, 132, 15795-15803.	2.0	40
180	Elucidation of Electron Ionization Induced Fragmentations of Adenine by Semiempirical and Density Functional Molecular Dynamics. Journal of Physical Chemistry A, 2014, 118, 11479-11484.	2.5	39

#	Article	IF	Citations
181	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.	3.0	38
182	Why Does the Intramolecular Trimethyleneâ€Bridged Frustrated Lewis Pair Mes₂PCH₂CH₂CH₂B(C₆F₅)₂ Not Activate Dihydrogen?. Chemistry - A European Journal, 2016, 22, 5988-5995.	3.3	37
183	S_N2 Reactions at Tertiary Carbon Centers in Epoxides. Angewandte Chemie - International Edition, 2017, 56, 9719-9722.	13.8	37
184	Electrophilic Phosphonium Cationâ€Mediated Phosphane Oxide Reduction Using Oxalyl Chloride and Hydrogen. Angewandte Chemie - International Edition, 2018, 57, 15253-15256.	13.8	37
185	Synthesis and Dynamics of Nanosized Phenyleneâ€"Ethynyleneâ€"Butadiynylene Rotaxanes and the Role of Shape Persistence. Angewandte Chemie - International Edition, 2016, 55, 3328-3333.	13.8	36
186	Oxâ€SLIM: Synthesis of and Siteâ€Specific Labelling with a Highly Hydrophilic Trityl Spin Label. Chemistry - A European Journal, 2021, 27, 5292-5297.	3.3	36
187	First principles calculation of electron ionization mass spectra for selected organic drug molecules. Organic and Biomolecular Chemistry, 2014, 12, 8737-8744.	2.8	35
188	Solid state frustrated Lewis pair chemistry. Chemical Science, 2018, 9, 4859-4865.	7.4	35
189	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.	5.3	34
190	Double FLP-Alkyne Exchange Reactions: A Facile Route to Te/B Heterocycles. Journal of the American Chemical Society, 2015, 137, 13264-13267.	13.7	34
191	Synthesis, Chiral Resolution, and Absolute Configuration of Dissymmetric 4,15-Difunctionalized [2.2]Paracyclophanes. Journal of Organic Chemistry, 2014, 79, 6679-6687.	3.2	33
192	Biomolecular Structure Information from High-Speed Quantum Mechanical Electronic Spectra Calculation. Journal of the American Chemical Society, 2017, 139, 11682-11685.	13.7	33
193	Calculation of Electron Ionization Mass Spectra with Semiempirical GFNn-xTB Methods. ACS Omega, 2019, 4, 15120-15133.	3.5	33
194	Quantum Chemical Calculation of Molecular and Periodic Peptide and Protein Structures. Journal of Physical Chemistry B, 2020, 124, 3636-3646.	2.6	33
195	Vollautomatisierte quantenchemische Berechnung von Spinâ€Spinâ€•gekoppelten magnetischen Kernspinresonanzspektren. Angewandte Chemie, 2017, 129, 14958-14964.	2.0	32
196	Formation of macrocyclic ring systems by carbonylation of trifunctional P/B/B frustrated Lewis pairs. Chemical Science, 2018, 9, 1544-1550.	7.4	32
197	Electrophilic Formylation of Arenes by Silylium Ion Mediated Activation of Carbon Monoxide. Angewandte Chemie - International Edition, 2018, 57, 8301-8305.	13.8	32
198	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.	5.3	32

#	Article	IF	Citations
199	Efficient Calculation of Small Molecule Binding in Metalâ€“Organic Frameworks and Porous Organic Cages. Journal of Physical Chemistry C, 2020, 124, 27529-27541.	3.1	32
200	Modeling of spinâ€“spin distance distributions for nitroxide labeled biomacromolecules. Physical Chemistry Chemical Physics, 2020, 22, 24282-24290.	2.8	32
201	Dispersion corrected r2SCAN based global hybrid functionals: r2SCANh, r2SCAN0, and r2SCAN50. Journal of Chemical Physics, 2022, 156, 134105.	3.0	32
202	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.	2.8	31
203	Benchmarking London dispersion corrected density functional theory for noncovalent ionâ€“Ï€ interactions. Physical Chemistry Chemical Physics, 2021, 23, 11635-11648.	2.8	31
204	Electronic Circular Dichroism of [16]Helicene With Simplified TDâ€DFT: Beyond the Single Structure Approach. Chirality, 2016, 28, 365-369.	2.6	30
205	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.	2.8	30
206	A Combined Experimental and Theoretical Study on the Conformation of Multiarmed Chiral Aryl Ethers. Journal of Organic Chemistry, 2007, 72, 6998-7010.	3.2	29
207	Frustrated Lewis pair addition to conjugated diynes: Formation of zwitterionic 1,2,3-butatriene derivatives. Dalton Transactions, 2012, 41, 9135.	3.3	29
208	Counterintuitive Interligand Angles in the Diaryls E{C₆H₃-2,6-(C₆H₂-2,4,6-^{<i>i</i>}Pr₃)₂}<sub (E = Ge, Sn, or Pb) and Related Species: The Role of London Dispersion Forces. Organometallics, 2018, 37, 2075-2085.	2.3	29
209	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.	13.8	29
210	What is the role of acidâ€“acid interactions in asymmetric phosphoric acid organocatalysis? A detailed mechanistic study using interlocked and non-interlocked catalysts. Chemical Science, 2020, 11, 4381-4390.	7.4	29
211	Chiral Dibenzopentaleneâ€Based Conjugated Nanohoops through Stereoselective Synthesis. Angewandte Chemie - International Edition, 2021, 60, 10680-10689.	13.8	29
212	Quantum Chemistry of FLPs and Their Activation of Small Molecules: Methodological Aspects. Topics in Current Chemistry, 2013, 332, 213-230.	4.0	28
213	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.	1.0	28
214	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
215	Coupling of Carbon Monoxide with Nitrogen Monoxide at a Frustrated Lewis Pair Template. Angewandte Chemie - International Edition, 2016, 55, 9216-9219.	13.8	28
216	The first microsolvation step for furans: New experiments and benchmarking strategies. Journal of Chemical Physics, 2020, 152, 164303.	3.0	28

#	Article	IF	Citations
217	Hochaktive Titanocenâ€Katalysatoren fÃ¼r Epoxidâ€Hydrosilylierungen â€“ Synthese, Theorie, Kinetik, EPRâ€Spektroskopie. Angewandte Chemie, 2016, 128, 7801-7805.	2.0	27
218	Halogen bonded supramolecular capsules: a challenging test case for quantum chemical methods. Chemical Communications, 2016, 52, 9893-9896.	4.1	26
219	Reversible formylborane/SO₂coupling at a frustrated Lewis pair framework. Chemical Communications, 2017, 53, 633-635.	4.1	26
220	Catalytic Difunctionalization of Unactivated Alkenes with Unreactive Hexamethyldisilane through Regeneration of Silylium Ions. Angewandte Chemie - International Edition, 2019, 58, 17307-17311.	13.8	26
221	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.	2.5	26
222	Selective Catalytic Frustrated Lewis Pair Hydrogenation of CO₂ in the Presence of Silylhalides. Angewandte Chemie - International Edition, 2021, 60, 25771-25775.	13.8	26
223	Boron Lewis Acid-Catalyzed Regioselective Hydrothiolation of Conjugated Dienes with Thiols. ACS Catalysis, 2019, 9, 11627-11633.	11.2	25
224	Folding of unstructured peptoids and formation of hetero-bimetallic peptoid complexes upon side-chain-to-metal coordination. Chemical Science, 2019, 10, 620-632.	7.4	25
225	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.	13.7	25
226	Far-IR and UV spectral signatures of controlled complexation and microhydration of the polycyclic aromatic hydrocarbon acenaphthene. Physical Chemistry Chemical Physics, 2019, 21, 3414-3422.	2.8	25
227	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.	3.0	25
228	Simplified time-dependent density functional theory (sTD-DFT) for molecular optical rotation. Journal of Chemical Physics, 2020, 153, 084116.	3.0	25
229	Quantification of Noncovalent Interactions in Azideâ€“Pnictogen, â€“Chalcogen, and â€“Halogen Contacts. Chemistry - A European Journal, 2021, 27, 4627-4639.	3.3	25
230	Ein praktikables rÃumliches MaÃŸ fÃ¼r Effekte statischer Elektronenkorrelation und deren Visualisierung. Angewandte Chemie, 2015, 127, 12483-12488.	2.0	24
231	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
232	Exhaustively Trichlorosilylated C₁ and C₂ Building Blocks: Beyond the MÃ¼llerâ€“Rochow Direct Process. Journal of the American Chemical Society, 2018, 140, 9696-9708.	13.7	23
233	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.	4.6	23
234	A Frustrated Phosphaneâ€“Borane Lewis Pair and Hydrogen: A Kinetics Study. Chemistry - A European Journal, 2016, 22, 11958-11961.	3.3	22

#	Article	IF	Citations
235	Trapping Experiments on a Trichlorosilanide Anion: a Key Intermediate of Halogenosilane Chemistry. Inorganic Chemistry, 2017, 56, 8683-8688.	4.0	22
236	Titanoceneâ€Catalyzed Radical Opening of Nâ€Acylated Aziridines. Angewandte Chemie, 2017, 129, 12828-12831.	2.0	22
237	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.	3.3	22
238	Calorimetric and quantum chemical studies of some photodimers of anthracenes. Physical Chemistry Chemical Physics, 1999, 1, 2457-2462.	2.8	21
239	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.	13.7	21
240	Structure Optimisation of Large Transitionâ€Metal Complexes with Extended Tightâ€Binding Methods. Angewandte Chemie, 2019, 131, 11195-11204.	2.0	21
241	The Chiral Trimer and a Metastable Chiral Dimer of Achiral Hexafluoroisopropanol: A Multiâ€Messenger Study. Angewandte Chemie, 2019, 131, 5134-5138.	2.0	20
242	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.	13.8	20
243	[Cl@Si₂₀H₂₀]^{âˆ’}: Parent Siladodecahedrane with Endohedral Chloride Ion. Journal of the American Chemical Society, 2021, 143, 10865-10871.	13.7	20
244	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.	7.4	19
245	Synthesis of 1,3â€Amino Alcohols by Hydroxyâ€Directed Aziridination and Aziridine Hydrosilylation. Angewandte Chemie - International Edition, 2018, 57, 13528-13532.	13.8	19
246	SET Oxidation of Li/X Phosphinidenoid Complexes by TEMPO. Organometallics, 2012, 31, 3457-3459.	2.3	18
247	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
248	Heterobifunctional Rotaxanes for Asymmetric Catalysis. Angewandte Chemie, 2020, 132, 5140-5145.	2.0	18
249	Fast and Accurate Quantum Chemical Modeling of Infrared Spectra of Condensed-Phase Systems. Journal of Physical Chemistry B, 2020, 124, 6664-6670.	2.6	18
250	Efficient Quantum-Chemical Calculations of Acid Dissociation Constants from Free-Energy Relationships. Journal of Physical Chemistry A, 2021, 125, 5681-5692.	2.5	18
251	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.	13.8	18
252	Automated Quantum Chemistry-Based Calculation of Optical Rotation for Large Flexible Molecules. Journal of Organic Chemistry, 2021, 86, 15522-15531.	3.2	18

#	Article	IF	Citations
253	Quantum Chemical Calculation and Evaluation of Partition Coefficients for Classical and Emerging Environmentally Relevant Organic Compounds. Environmental Science & Technology, 2022, 56, 379-391.	10.0	18
254	Accurate Thermochemistry for Large Molecules with Modern Density Functionals. Topics in Current Chemistry, 2014, , 1-23.	4.0	17
255	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
256	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.	13.7	17
257	Synthesis and Rearrangement of <i>P</i>â€Nitroxylâ€Substituted P^{III} and P^V Phosphanes: A Combined Experimental and Theoretical Case Study. Chemistry - A European Journal, 2016, 22, 10102-10110.	3.3	16
258	Computerchemie: das Schicksal aktueller Methoden und zukÃ¼nftige Herausforderungen. Angewandte Chemie, 2018, 130, 4241-4248.	2.0	16
259	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.	3.3	16
260	Reduction of Phosphine Oxide by Using Chlorination Reagents and Dihydrogen: DFT Mechanistic Insights. Chemistry - A European Journal, 2019, 25, 4670-4672.	3.3	16
261	Revisiting conformations of methyl lactate in water and methanol. Journal of Chemical Physics, 2021, 155, 024507.	3.0	16
262	Conformational Energy Benchmark for Longer <i>n</i>-Alkane Chains. Journal of Physical Chemistry A, 2022, 126, 3521-3535.	2.5	16
263	The inhibition of iridium-promoted water oxidation catalysis (WOC) by cucurbit[n]urils. Dalton Transactions, 2012, 41, 12233.	3.3	15
264	Perspective on Simplified Quantum Chemistry Methods for Excited States and Response Properties. Journal of Physical Chemistry A, 2021, 125, 3841-3851.	2.5	15
265	Facile Synthesis of Cyanide and Isocyanides from CO. Angewandte Chemie - International Edition, 2021, 60, 16965-16969.	13.8	15
266	Towards understanding solvation effects on the conformational entropy of non-rigid molecules. Physical Chemistry Chemical Physics, 2022, 24, 12249-12259.	2.8	15
267	The Role of Packing, Dispersion, Electrostatics, and Solvation in Highâ€Affinity Complexes of Cucurbit[<i>n</i>]urils with Uncharged Polar Guests. Chemistry - A European Journal, 2022, 28, .	3.3	15
268	Strong Evidence of a Phosphanoxyl Complex: Formation, Bonding, and Reactivity of Ligated Phosphorus Analogues of Nitroxides. Angewandte Chemie - International Edition, 2016, 55, 14439-14443.	13.8	14
269	Frustrated Lewis Pair Catalyzed Reduction of Carbon Dioxide Using Hydroboranes: New DFT Mechanistic Insights. ChemCatChem, 2020, 12, 3656-3660.	3.7	14
270	Comprehensive Benchmark Study on the Calculation of ²⁹Si NMR Chemical Shifts. Inorganic Chemistry, 2021, 60, 272-285.	4.0	14

#	Article	IF	Citations
271	Titanoceneâ€Catalyzed [2+2] Cycloaddition of Bisenones and Comparison with Photoredox Catalysis and Established Methods. Angewandte Chemie - International Edition, 2021, 60, 14339-14344.	13.8	14
272	Selective phosphanyl complex trapping using TEMPO. Synthesis and reactivity of P-functional P-nitroxyl phosphane complexes. Chemical Communications, 2014, 50, 12508-12511.	4.1	13
273	Cyclic Amine/Borane Lewis Pairs by the Reaction of <i>N</i>,<i>N</i>â€Diallylaniline with Lancasterâ€²s H₂Bâ€C₆F₅ Reagent. Chemistry - an Asian Journal, 2016, 11, 1394-1399.	3.3	13
274	Synthesis and Comprehensive Structural and Chiroptical Characterization of Enones Derived from (âˆ’)-Î±-Santonin by Experiment and Theory. Journal of Organic Chemistry, 2016, 81, 4588-4600.	3.2	13
275	Unimolecular decomposition pathways of negatively charged nitriles by ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2016, 18, 31017-31026.	2.8	13
276	S_N2 Reactions at Tertiary Carbon Centers in Epoxides. Angewandte Chemie, 2017, 129, 9851-9854.	2.0	13
277	Dynamic Structural Effects on the Second-Harmonic Generation of Tryptophane-Rich Peptides and Gramicidin A. Journal of Physical Chemistry B, 2020, 124, 2568-2578.	2.6	13
278	Boron-Catalyzed Hydroarylation of 1,3-Dienes with Arylamines. Organic Letters, 2021, 23, 8952-8957.	4.6	13
279	Increased Antiaromaticity through Pentalene Connection in [<i>n</i>]Cyclo-1,5-dibenzopentalenes. Organic Letters, 2022, 24, 983-988.	4.6	13
280	Theoretical Study of the Stacking Behavior of Selected Polycondensed Aromatic Hydrocarbons with Various Symmetries. Journal of Physical Chemistry A, 2013, 117, 616-625.	2.5	12
281	Aggregation Behavior of a Sixâ€Membered Cyclic Frustrated Phosphane/Borane Lewis Pair: Formation of a Supramolecular Cyclooctameric Macrocyclic Ring System. Angewandte Chemie, 2019, 131, 892-896.	2.0	12
282	Influencing the Selfâ€Sorting Behavior of [2.2]Paracyclophaneâ€Based Ligands by Introducing Isostructural Binding Motifs. Chemistry - A European Journal, 2020, 26, 3335-3347.	3.3	12
283	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.	3.0	12
284	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.	0.8	12
285	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.	3.3	12
286	Intermolecular Carbosilylation of Î±â€Olefins with C(sp3)â€"C(sp) Bond Formation Involving Silyliumâ€Ion Regeneration. Angewandte Chemie - International Edition, 2022, , .	13.8	12
287	Elektrophile Formylierung von Aromaten durch silyliumionvermittelte Aktivierung von Kohlenmonoxid. Angewandte Chemie, 2018, 130, 8433-8437.	2.0	11
288	A Unified Strategy for the Chemically Intuitive Interpretation of Molecular Optical Response Properties. Journal of Chemical Theory and Computation, 2020, 16, 7709-7720.	5.3	11

#	Article	IF	Citations
289	Mechanistic Insights for Nitromethane Activation into Reactive Nitrogenating Reagents. ChemCatChem, 2021, 13, 2132-2137.	3.7	11
290	Frustrated Lewis pair catalyzed hydrodehalogenation of benzyl-halides. Chemical Communications, 2022, 58, 1175-1178.	4.1	11
291	Benchmark Study on the Calculation of ¹¹⁹Sn NMR Chemical Shifts. Inorganic Chemistry, 2022, 61, 3903-3917.	4.0	11
292	Chemistry of Thermally Generated Transient Phosphanoxyl Complexes. Organometallics, 2017, 36, 2877-2883.	2.3	10
293	Thermodynamics of H⁺/H^{â€¢}/H^{â€“}/e^{â€“} Transfer from [CpV(CO)₃H]^{âˆ’}: Comparisons to the Isoelectronic CpCr(CO)₃H. Organometallics, 2019, 38, 4319-4328.	2.3	10
294	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.	3.3	10
295	Boraneâ€Catalyzed Hydrogenation of Tertiary Amides Activated by Oxalyl Chloride: DFT Mechanistic Insights. European Journal of Organic Chemistry, 2019, 2019, 4609-4612.	2.4	10
296	Acidâ€Catalyzed Rearrangements of 3â€Aryloxiraneâ€2â€Carboxamides: Novel DFT Mechanistic Insights. ChemistryOpen, 2020, 9, 743-747.	1.9	10
297	Oxidation Under Reductive Conditions: From Benzylic Ethers to Acetals with Perfect Atomâ€Economy by Titanocene(III) Catalysis. Angewandte Chemie, 2021, 133, 5542-5548.	2.0	10
298	Hydrocarbon Macrocycle Conformer Ensembles and ¹³Câ€NMR Spectra. Angewandte Chemie - International Edition, 2022, 61, .	13.8	10
299	Synthesis, Chiral Resolution, and Absolute Configuration of Functionalized TrÃ¶gerâ€™s Base Derivatives: Part III. Synthesis, 2015, 47, 3118-3132.	2.3	9
300	transâ€“cis Câ€“Pdâ€“C rearrangement in hemichelates. Dalton Transactions, 2017, 46, 8125-8137.	3.3	9
301	Acylation Reactions of Dibenzoâ€7â€phosphanorbornadiene: DFT Mechanistic Insights. ChemistryOpen, 2019, 8, 807-810.	1.9	9
302	Mechanistic Insights for Dimethyl Sulfoxide Catalyzed Aromatic Chlorination Reactions. ChemCatChem, 2021, 13, 207-211.	3.7	9
303	Chiral Dibenzopentaleneâ€Based Conjugated Nanohoops through Stereoselective Synthesis. Angewandte Chemie, 2021, 133, 10775-10784.	2.0	9
304	LiAlH 4 â€catalyzed Imine Hydrogenation with Dihydrogen: New DFT Mechanistic Insights. ChemCatChem, 2021, 13, 3401-3404.	3.7	9
305	Hydrogenation of Secondary Amides using Phosphane Oxide and Frustrated Lewis Pair Catalysis. Chemistry - A European Journal, 2021, 27, 14179-14183.	3.3	9
306	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

#	Article	IF	Citations
307	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.	3.4	8
308	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.	2.4	8
309	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.	13.8	8
310	Nanoscale Ï€-conjugated ladders. Nature Communications, 2021, 12, 6614.	12.8	8
311	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, .	3.3	8
312	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.	2.5	8
313	Reduktion von Phosphanoxiden mit Oxalylchlorid und Wasserstoff, vermittelt durch ein elektrophiles Phosphoniumkation. Angewandte Chemie, 2018, 130, 15473-15476.	2.0	7
314	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.	2.8	7
315	Steric Influence on Reactions of Benzyl Potassium Species with CO. Chemistry - an Asian Journal, 2021, 16, 3640-3644.	3.3	7
316	Synthesis and Mechanistic Insights of the Formation of 3-Hydroxyquinolin-2-ones including Viridicatin from 2-Chloro-<i>N</i>,3-diaryloxirane-2-carboxamides under Acid-Catalyzed Rearrangements. Journal of Organic Chemistry, 2021, 86, 13514-13534.	3.2	7
317	Nanopatterns of molecular spoked wheels as giant homologues of benzene tricarboxylic acids. Chemical Science, 2021, 12, 9352-9358.	7.4	7
318	Selective catalytic Frustrated Lewis Pair Hydrogenation of CO2 in the Presence of Silylhalides. Angewandte Chemie, 2021, 133, 25975.	2.0	7
319	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.	13.8	6
320	Ligand Protonation at Carbon, not Nitrogen, during H₂ Production with Amine-Rich Iron Electrocatalysts. Inorganic Chemistry, 2021, 60, 17407-17413.	4.0	6
321	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.	13.7	6
322	Are Fully Conjugated Expanded Indenofluorenes Analogues and Diindeno[<i>n</i>]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.	2.5	5
323	Katalytische Difunktionalisierung von nichtaktivierten Alkenen mit reaktionstrÃ¤gem Hexamethyldisilan durch Neubildung von Silyliumionen. Angewandte Chemie, 2019, 131, 17468-17472.	2.0	5
324	Mechanistic Insights for Anilineâ€Catalyzed Halogenation Reactions. ChemCatChem, 2020, 12, 5369-5373.	3.7	5

#	Article	IF	Citations
325	Mechanistic Insights for Iodane Mediated Aromatic Halogenation Reactions. ChemCatChem, 2020, 12, 6186-6190.	3.7	5
326	Mechanistic Insights for Acidâ€catalyzed Rearrangement of Quinoxalinâ€2â€one with Diamine and Enamine. ChemCatChem, 2021, 13, 1503-1508.	3.7	5
327	Reactions of a Dilithiomethane with CO and N₂O: An Avenue to an Anionic Ketene and a Hexafunctionalized Benzene. Angewandte Chemie, 2021, 133, 25485-25489.	2.0	5
328	All-Atom Quantum Mechanical Calculation of the Second-Harmonic Generation of Fluorescent Proteins. Journal of Physical Chemistry Letters, 2021, 12, 9684-9690.	4.6	5
329	Hydrogen atom transfer rates from Tp-containing metal-hydrides to trityl radicals. Canadian Journal of Chemistry, 2021, 99, 216-220.	1.1	5
330	HFIPâ€Assisted Single Câˆ’F Bond Activation of Trifluoromethyl Ketones using Visibleâ€Light Photoredox Catalysis. Angewandte Chemie, 2022, 134, .	2.0	5
331	Starker Hinweis auf einen Phosphanoxylkomplex: Bildung, Bindung und ReaktivitÃt komplexgebundener Pâ€Analoga von Nitroxiden. Angewandte Chemie, 2016, 128, 14654-14658.	2.0	4
332	Synthesis of 1,3â€Amino Alcohols by Hydroxyâ€Directed Aziridination and Aziridine Hydrosilylation. Angewandte Chemie, 2018, 130, 13716-13720.	2.0	4
333	Extension of the element parameter set for ultra-fast excitation spectra calculation (sTDA-xTB). Molecular Physics, 2019, 117, 1104-1116.	1.7	4
334	The power of trichlorosilylation: isolable trisilylated allyl anions, allyl radicals, and allenyl anions. Chemical Science, 2021, 12, 12419-12428.	7.4	4
335	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.	2.0	4
336	Titanoceneâ€Catalyzed [2+2] Cycloaddition of Bisenones and Comparison with Photoredox Catalysis and Established Methods. Angewandte Chemie, 2021, 133, 14460-14465.	2.0	4
337	Facile Synthesis of Cyanide and Isocyanides from CO. Angewandte Chemie, 2021, 133, 17102-17106.	2.0	4
338	High-Throughput Non-targeted Chemical Structure Identification Using Gas-Phase Infrared Spectra. Analytical Chemistry, 2021, 93, 10688-10696.	6.5	4
339	Supramolecular Nanopatterns of Molecular Spoked Wheels with Orthogonal Pillars: The Observation of a Fullerene Haze. Angewandte Chemie - International Edition, 2021, 60, 27264-27270.	13.8	4
340	The Nonâ€Ancillary Nature of Trimethylsilylamide Substituents in Boranes and Borinium Cations. Chemistry - A European Journal, 2022, 28, .	3.3	4
341	Quickstart guide to model structures and interactions of artificial molecular muscles with efficient computational methods. Chemical Communications, 2021, 58, 258-261.	4.1	3
342	Catalytic Isomerization of Unprotected Mesoionic <i>N</i>â€Heterocyclic Olefins and Their Lewis Adducts. European Journal of Organic Chemistry, 2022, 2022, .	2.4	3

#	Article	IF	Citations
343	Stoichiometric and catalytic isomerization of alkenylboranes using bulky Lewis bases. Chemical Communications, 2017, 53, 9458-9461.	4.1	2
344	Structural and Conformational Studies on Carboxamides of 5,6-Diaminouracilsâ€"Precursors of Biologically Active Xanthine Derivatives. Molecules, 2019, 24, 2168.	3.8	2
345	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.	2.0	2
346	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.	3.3	2
347	Stereochemical Behavior of Pairs of Pâ€stereogenic Phosphanyl Groups at the Dimethylxanthene Backbone. Chemistry - A European Journal, 2022, , .	3.3	2
348	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, , .	3.7	2
349	Sensory Perception of Nonâ€Deuterated and Deuterated Organic Compounds. Chemistry - A European Journal, 2021, 27, 1046-1056.	3.3	1
350	Supramolecular Nanopatterns of Molecular Spoked Wheels with Orthogonal Pillars: The Observation of a Fullerene Haze. Angewandte Chemie, 0, , .	2.0	1
351	Hydrocarbon Macrocycle Conformer Ensembles and 13Câ€NMR spectra. Angewandte Chemie, 0, , .	2.0	1
352	The long-awaited synthesis and self-assembly of a small rigid <i>C</i>₃-symmetric trilactam. Chemical Communications, 2022, 58, 3751-3754.	4.1	1
353	Computational study of groundâ€state properties of <i>Î¼</i> ₂ â€bridged group 14 porphyrinic sandwich complexes. Journal of Computational Chemistry, 2022, , .	3.3	1
354	Catalyst-free CO₂ hydrogenation with BH₃NH₃ in water: DFT mechanistic insights. Physical Chemistry Chemical Physics, 2022, 24, 14159-14164.	2.8	1
355	Titelbild: Supramolecular Nanopatterns of Molecular Spoked Wheels with Orthogonal Pillars: The Observation of a Fullerene Haze (Angew. Chem. 52/2021). Angewandte Chemie, 2021, 133, 27073-27073.	2.0	0
356	Intermolecular Carbosilylation of Î±â€Olefins with C(sp3)â€"C(sp) Bond Formation Involving Silyliumâ€Ion Regeneration. Angewandte Chemie, 0, , .	2.0	0
357	Acidâ€Catalyzed Carbene Transfer from Diazo Compounds: Carbocation versus Carbene as Key Intermediate. European Journal of Organic Chemistry, 0, , .	2.4	0