

# Stefan Grimme

## List of Publications by Year in descending order

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357  
papers

128,975  
citations

2311

98  
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102

350  
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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. <i>Journal of Chemical Physics</i> , 2010, 132, 154104.	1.2	35,972
2	Semiempirical GGA-type density functional constructed with a long-range dispersion correction. <i>Journal of Computational Chemistry</i> , 2006, 27, 1787-1799.	1.5	24,222
3	Effect of the damping function in dispersion corrected density functional theory. <i>Journal of Computational Chemistry</i> , 2011, 32, 1456-1465.	1.5	15,980
4	Accurate description of van der Waals complexes by density functional theory including empirical corrections. <i>Journal of Computational Chemistry</i> , 2004, 25, 1463-1473.	1.5	4,372
5	Semiempirical hybrid density functional with perturbative second-order correlation. <i>Journal of Chemical Physics</i> , 2006, 124, 034108.	1.2	2,729
6	Density functional theory with London dispersion corrections. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011, 1, 211-228.	6.2	2,030
7	GFN2-xTB: An Accurate and Broadly Parametrized Self-Consistent Tight-Binding Quantum Chemical Method with Multipole Electrostatics and Density-Dependent Dispersion Contributions. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1652-1671.	2.3	1,704
8	A thorough benchmark of density functional methods for general main group thermochemistry, kinetics, and noncovalent interactions. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 6670.	1.3	1,627
9	Improved second-order Møller-Plesset perturbation theory by separate scaling of parallel- and antiparallel-spin pair correlation energies. <i>Journal of Chemical Physics</i> , 2003, 118, 9095-9102.	1.2	1,607
10	Supramolecular Binding Thermodynamics by Dispersion-Corrected Density Functional Theory. <i>Chemistry - A European Journal</i> , 2012, 18, 9955-9964.	1.7	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. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 32184-32215.	1.3	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 ( $Z \leq 86$ ). <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1989-2009.	2.3	1,072
13	Efficient and Accurate Double-Hybrid-Meta-GGA Density Functionals: Evaluation with the Extended GMTKN30 Database for General Main Group Thermochemistry, Kinetics, and Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 291-309.	2.3	1,035
14	Dispersion-Corrected Mean-Field Electronic Structure Methods. <i>Chemical Reviews</i> , 2016, 116, 5105-5154.	23.0	1,032
15	Double-hybrid density functionals with long-range dispersion corrections: higher accuracy and extended applicability. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 3397.	1.3	979
16	Automated exploration of the low-energy chemical space with fast quantum chemical methods. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 7169-7192.	1.3	966
17	Do Special Noncovalent $\pi$ - $\pi$ Stacking Interactions Really Exist?. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 3430-3434.	7.2	928
18	A generally applicable atomic-charge dependent London dispersion correction. <i>Journal of Chemical Physics</i> , 2019, 150, 154122.	1.2	697

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19	Density functional theory with dispersion corrections for supramolecular structures, aggregates, and complexes of (bio)organic molecules. <i>Organic and Biomolecular Chemistry</i> , 2007, 5, 741-758.	1.5	683
20	Reversible Metal-Free Carbon Dioxide Binding by Frustrated Lewis Pairs. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 6643-6646.	7.2	680
21	A combination of Kohn-Sham density functional theory and multi-reference configuration interaction methods. <i>Journal of Chemical Physics</i> , 1999, 111, 5645-5655.	1.2	635
22	Extension of the D3 dispersion coefficient model. <i>Journal of Chemical Physics</i> , 2017, 147, 034112.	1.2	617
23	Consistent structures and interactions by density functional theory with small atomic orbital basis sets. <i>Journal of Chemical Physics</i> , 2015, 143, 054107.	1.2	605
24	Extended tight-binding quantum chemistry methods. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, e1493.	6.2	596
25	Rapid intramolecular heterolytic dihydrogen activation by a four-membered heterocyclic phosphane-borane adduct. <i>Chemical Communications</i> , 2007, , 5072.	2.2	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. <i>Journal of Chemical Physics</i> , 2012, 136, 154101.	1.2	556
27	Exploration of Chemical Compound, Conformer, and Reaction Space with Meta-Dynamics Simulations Based on Tight-Binding Quantum Chemical Calculations. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2847-2862.	2.3	551
28	Towards chemical accuracy for the thermodynamics of large molecules: new hybrid density functionals including non-local correlation effects. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 4398.	1.3	538
29	DFT-D3 Study of Some Molecular Crystals. <i>Journal of Physical Chemistry C</i> , 2014, 118, 7615-7621.	1.5	457
30	Report on the sixth blind test of organic crystal structure prediction methods. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 439-459.	0.5	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. <i>Journal of Organic Chemistry</i> , 2012, 77, 10824-10834.	1.7	407
32	Double-hybrid density functional theory for excited electronic states of molecules. <i>Journal of Chemical Physics</i> , 2007, 127, 154116.	1.2	404
33	B97-3c: A revised low-cost variant of the B97-D density functional method. <i>Journal of Chemical Physics</i> , 2018, 148, 064104.	1.2	400
34	The Mechanism of Dihydrogen Activation by Frustrated Lewis Pairs Revisited. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 1402-1405.	7.2	394
35	A General Database for Main Group Thermochemistry, Kinetics, and Noncovalent Interactions - Assessment of Common and Reparameterized (meta-GGA) Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 107-126.	2.3	389
36	Benchmarking of London Dispersion-Accounting Density Functional Theory Methods on Very Large Molecular Complexes. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1580-1591.	2.3	362

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37	Seemingly Simple Stereoelectronic Effects in Alkane Isomers and the Implications for Kohn-Sham Density Functional Theory. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 4460-4464.	7.2	360
38	Corrected small basis set Hartree-Fock method for large systems. <i>Journal of Computational Chemistry</i> , 2013, 34, 1672-1685.	1.5	358
39	Theoretical Thermodynamics for Large Molecules: Walking the Thin Line between Accuracy and Computational Cost. <i>Accounts of Chemical Research</i> , 2008, 41, 569-579.	7.6	329
40	System-Dependent Dispersion Coefficients for the DFT-D3 Treatment of Adsorption Processes on Ionic Surfaces. <i>ChemPhysChem</i> , 2011, 12, 3414-3420.	1.0	318
41	Double-hybrid density functionals. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2014, 4, 576-600.	6.2	292
42	r2SCAN-3c: A "Swiss army knife"-composite electronic-structure method. <i>Journal of Chemical Physics</i> , 2021, 154, 064103.	1.2	290
43	Benchmarking Density Functional Methods against the S66 and S66x8 Datasets for Non-Covalent Interactions. <i>ChemPhysChem</i> , 2011, 12, 3421-3433.	1.0	283
44	Full Selectivity Control in Cobalt(III)-Catalyzed C-H Alkylations by Switching of the C-H Activation Mechanism. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 10378-10382.	7.2	243
45	A simplified Tamm-Dancoff density functional approach for the electronic excitation spectra of very large molecules. <i>Journal of Chemical Physics</i> , 2013, 138, 244104.	1.2	242
46	Accurate Calculation of the Heats of Formation for Large Main Group Compounds with Spin-Component Scaled MP2 Methods. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3067-3077.	1.1	241
47	Effects of London dispersion correction in density functional theory on the structures of organic molecules in the gas phase. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 16031.	1.3	238
48	How to Compute Isomerization Energies of Organic Molecules with Quantum Chemical Methods. <i>Journal of Organic Chemistry</i> , 2007, 72, 2118-2126.	1.7	234
49	Steric Crowding Can Stabilize a Labile Molecule: Solving the Hexaphenylethane Riddle. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 12639-12642.	7.2	232
50	Metal-free Catalytic Olefin Hydrogenation: Low-Temperature H <sub>2</sub> -Activation by Frustrated Lewis Pairs. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 10164-10168.	7.2	230
51	Robust Atomistic Modeling of Materials, Organometallic, and Biochemical Systems. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 15665-15673.	7.2	224
52	Reactions of an Intramolecular Frustrated Lewis Pair with Unsaturated Substrates: Evidence for a Concerted Olefin Addition Reaction. <i>Journal of the American Chemical Society</i> , 2009, 131, 12280-12289.	6.6	218
53	"Mindless"-DFT Benchmarking. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 993-1003.	2.3	215
54	Performance of the van der Waals Density Functional VV10 and (hybrid)GGA Variants for Thermochemistry and Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3866-3871.	2.3	213

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55	A simplified time-dependent density functional theory approach for electronic ultraviolet and circular dichroism spectra of very large molecules. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 45-53.	1.1	211
56	Performance of dispersion-corrected density functional theory for the interactions in ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 4875.	1.3	202
57	Comprehensive Thermochemical Benchmark Set of Realistic Closed-Shell Metal Organic Reactions. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2596-2608.	2.3	202
58	Assessment of Orbital-Optimized, Spin-Component Scaled Second-Order Many-Body Perturbation Theory for Thermochemistry and Kinetics. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 3060-3073.	2.3	199
59	Spin-component-scaled electron correlation methods. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2012, 2, 886-906.	6.2	197
60	A Practicable Real-Space Measure and Visualization of Static Electron-Correlation Effects. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 12308-12313.	7.2	194
61	An improved method for density functional calculations of the frequency-dependent optical rotation. <i>Chemical Physics Letters</i> , 2002, 361, 321-328.	1.2	189
62	On the Importance of the Dispersion Energy for the Thermodynamic Stability of Molecules. <i>ChemPhysChem</i> , 2011, 12, 1258-1261.	1.0	188
63	Comprehensive Benchmark of Association (Free) Energies of Realistic Host-Guest Complexes. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3785-3801.	2.3	188
64	Robust and Efficient Implicit Solvation Model for Fast Semiempirical Methods. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4250-4261.	2.3	186
65	Capture of NO by a Frustrated Lewis Pair: A New Type of Persistent <i>N</i> -Oxyl Radical. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 7567-7571.	7.2	181
66	Combinations of Ethers and B(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> Function as Hydrogenation Catalysts. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 7492-7495.	7.2	180
67	Reaction of Frustrated Lewis Pairs with Conjugated Ynones-Selective Hydrogenation of the Carbon-Carbon Triple Bond. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 7183-7186.	7.2	169
68	C-F/C-H Functionalization by Manganese(I) Catalysis: Expedient (Per)Fluoro-Allylations and Alkenylations. <i>ACS Catalysis</i> , 2017, 7, 4209-4213.	5.5	165
69	Is Spin-Component Scaled Second-Order Møller-Plesset Perturbation Theory an Appropriate Method for the Study of Noncovalent Interactions in Molecules?. <i>Journal of Physical Chemistry A</i> , 2007, 111, 4862-4868.	1.1	164
70	On the Importance of Electron Correlation Effects for the $\pi$ - $\pi$ Interactions in Cyclophanes. <i>Chemistry - A European Journal</i> , 2004, 10, 3423-3429.	1.7	162
71	Calculation of frequency dependent optical rotation using density functional response theory. <i>Chemical Physics Letters</i> , 2001, 339, 380-388.	1.2	158
72	Fully Automated Quantum-Chemistry-Based Computation of Spin-Coupled Nuclear Magnetic Resonance Spectra. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 14763-14769.	7.2	158

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73	Accurate Modeling of Organic Molecular Crystals by Dispersion-Corrected Density Functional Tight Binding (DFTB). <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 1785-1789.	2.1	155
74	A General Quantum Mechanically Derived Force Field (QMDF) for Molecules and Condensed Phase Simulations. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4497-4514.	2.3	154
75	<i>N</i> , <i>N</i> -Addition of Frustrated Lewis Pairs to Nitric Oxide: An Easy Entry to a Unique Family of Aminoxy Radicals. <i>Journal of the American Chemical Society</i> , 2012, 134, 10156-10168.	6.6	153
76	Reactions of phosphorus/boron frustrated Lewis pairs with SO <sub>2</sub> . <i>Chemical Science</i> , 2013, 4, 213-219.	3.7	150
77	Towards First Principles Calculation of Electron Impact Mass Spectra of Molecules. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 6306-6312.	7.2	148
78	CO <sub>2</sub> and Formate Complexes of Phosphine/Borane Frustrated Lewis Pairs. <i>Chemistry - A European Journal</i> , 2011, 17, 9640-9650.	1.7	146
79	Benchmark Study of the Performance of Density Functional Theory for Bond Activations with (Ni,Pd)-Based Transition-Metal Catalysts. <i>ChemistryOpen</i> , 2013, 2, 115-124.	0.9	146
80	Facile Carbon Monoxide Reduction at Intramolecular Frustrated Phosphane/Borane Lewis Pair Templates. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 2243-2246.	7.2	143
81	Computational Chemistry: The Fate of Current Methods and Future Challenges. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 4170-4176.	7.2	138
82	Extension and evaluation of the D4 London-dispersion model for periodic systems. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 8499-8512.	1.3	138
83	Mechanism of Titanocene-Mediated Epoxide Opening through Homolytic Substitution. <i>Journal of the American Chemical Society</i> , 2007, 129, 1359-1371.	6.6	135
84	Cation-Cation $\pi$ -Attraction: When London Dispersion Attraction Wins over Coulomb Repulsion. <i>Inorganic Chemistry</i> , 2011, 50, 2619-2628.	1.9	127
85	London Dispersion Enables the Shortest Intermolecular Hydrocarbon H $\cdots$ H Contact. <i>Journal of the American Chemical Society</i> , 2017, 139, 7428-7431.	6.6	126
86	Formation of Cyclic Allenes and Cumulenes by Cooperative Addition of Frustrated Lewis Pairs to Conjugated Enynes and Diynes. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 2414-2417.	7.2	125
87	Using dispersion-corrected density functional theory to understand supramolecular binding thermodynamics. <i>Chemical Communications</i> , 2015, 51, 1764-1774.	2.2	125
88	Effects of London dispersion on the isomerization reactions of large organic molecules: a density functional benchmark study. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6940.	1.3	123
89	Geometrical Correction for the Inter- and Intramolecular Basis Set Superposition Error in Periodic Density Functional Theory Calculations. <i>Journal of Physical Chemistry A</i> , 2013, 117, 9282-9292.	1.1	123
90	Improved third-order Møller-Plesset perturbation theory. <i>Journal of Computational Chemistry</i> , 2003, 24, 1529-1537.	1.5	117

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91	Understanding and Quantifying London Dispersion Effects in Organometallic Complexes. <i>Accounts of Chemical Research</i> , 2019, 52, 258-266.	7.6	117
92	Importance of London dispersion effects for the packing of molecular crystals: a case study for intramolecular stacking in a bis-thiophene derivative. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 8500.	1.3	115
93	Ultra-fast computation of electronic spectra for large systems by tight-binding based simplified Tamm-Dancoff approximation (sTDA-xTB). <i>Journal of Chemical Physics</i> , 2016, 145, 054103.	1.2	115
94	A Radical Tandem Reaction with Homolytic Cleavage of a Ti- $\eta^5$ -O Bond. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 3687-3690.	7.2	110
95	Exploring the Limits of Frustrated Lewis Pair Chemistry with Alkynes: Detection of a System that Favors 1,1-Carboboration over Cooperative 1,2- $\pi$ - $\pi$ Addition. <i>Chemistry - an Asian Journal</i> , 2010, 5, 2199-2208.	1.7	106
96	Efficient Quantum Chemical Calculation of Structure Ensembles and Free Energies for Nonrigid Molecules. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4039-4054.	1.1	105
97	Calculation of the Electronic Spectra of Large Molecules. <i>Reviews in Computational Chemistry</i> , 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. <i>Chemistry - A European Journal</i> , 2017, 23, 6150-6164.	1.7	102
99	Enantiomerically Pure [M <sub>6</sub> L <sub>12</sub> ] or [M <sub>12</sub> L <sub>24</sub> ] Polyhedra from Flexible Bis(Pyridine) Ligands. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 1693-1698.	7.2	96
100	Consistent Theoretical Description of 1,3-Dipolar Cycloaddition Reactions. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2583-2586.	1.1	95
101	Full Selectivity Control in Cobalt(III)-Catalyzed C-H Alkylations by Switching of the C-H Activation Mechanism. <i>Angewandte Chemie</i> , 2017, 129, 10514-10518.	1.6	95
102	Mild Cobalt(III)-Catalyzed Allylative C-F/C-H Functionalizations at Room Temperature. <i>Chemistry - A European Journal</i> , 2017, 23, 12145-12148.	1.7	95
103	Carbonylation Reactions of Intramolecular Vicinal Frustrated Phosphane/Borane Lewis Pairs. <i>Journal of the American Chemical Society</i> , 2013, 135, 18567-18574.	6.6	94
104	Electronic effects of triarylphosphines in metal-free hydrogen activation: a kinetic and computational study. <i>Chemical Science</i> , 2013, 4, 2788.	3.7	93
105	1,1-Hydroboration and a Borane Adduct of Diphenyldiazomethane: A Potential Prelude to FLP $\pi$ - $\pi$ Chemistry. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 16588-16592.	7.2	93
106	Performance of Non-Local and Atom-Pairwise Dispersion Corrections to DFT for Structural Parameters of Molecules with Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 308-315.	2.3	91
107	Quantum Chemical Benchmark Study on 46 RNA Backbone Families Using a Dinucleotide Unit. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4972-4991.	2.3	90
108	Elucidation of the Mechanism of Titanocene-Mediated Epoxide Opening by a Combined Experimental and Theoretical Approach. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 2041-2044.	7.2	89

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109	How to Compute Electron Ionization Mass Spectra from First Principles. <i>Journal of Physical Chemistry A</i> , 2016, 120, 3755-3766.	1.1	88
110	Functional Mechanically Interlocked Molecules: Asymmetric Organocatalysis with a Catenated Bifunctional Brønsted Acid. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 11456-11459.	7.2	88
111	Exploration of the Solid-State Sorption Properties of Shape-Persistent Macrocyclic Nanocarbons as Bulk Materials and Small Aggregates. <i>Journal of the American Chemical Society</i> , 2020, 142, 8763-8775.	6.6	86
112	Benchmarking DFT and semiempirical methods on structures and lattice energies for ten ice polymorphs. <i>Journal of Chemical Physics</i> , 2015, 142, 124104.	1.2	84
113	Calculation of absolute molecular entropies and heat capacities made simple. <i>Chemical Science</i> , 2021, 12, 6551-6568.	3.7	83
114	Remarkable coordination behavior of alkyl isocyanides toward unsaturated vicinal frustrated P/B Lewis pairs. <i>Chemical Science</i> , 2013, 4, 2657.	3.7	81
115	1,1-Hydroboration and a Borane Adduct of Diphenyldiazomethane: A Potential Prelude to FLP Chemistry. <i>Angewandte Chemie</i> , 2017, 129, 16815-16819.	1.6	81
116	Low-Cost Quantum Chemical Methods for Noncovalent Interactions. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 4275-4284.	2.1	80
117	B(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> -Catalyzed Transfer of Dihydrogen from One Unsaturated Hydrocarbon to Another. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 12158-12162.	7.2	80
118	An Octanuclear Metallocuprate Cage Designed To Exhibit Spin-Crossover Behavior. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 4930-4935.	7.2	80
119	Quantum chemical calculation of electron ionization mass spectra for general organic and inorganic molecules. <i>Chemical Science</i> , 2017, 8, 4879-4895.	3.7	79
120	Protein-Ligand Interaction Energies with Dispersion Corrected Density Functional Theory and High-Level Wave Function Based Methods. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11210-11220.	1.1	78
121	New Insights into Frustrated Lewis Pairs: Structural Investigations of Intramolecular Phosphane-Borane Adducts by Using Modern Solid-State NMR Techniques and DFT Calculations. <i>Journal of the American Chemical Society</i> , 2012, 134, 4236-4249.	6.6	78
122	Substituent Effects and Supramolecular Interactions of Titanocene(III) Chloride: Implications for Catalysis in Single Electron Steps. <i>Journal of the American Chemical Society</i> , 2014, 136, 1663-1671.	6.6	78
123	Hydrosilylation of Ketones, Imines and Nitriles Catalysed by Electrophilic Phosphonium Cations: Functional Group Selectivity and Mechanistic Considerations. <i>Chemistry - A European Journal</i> , 2015, 21, 6491-6500.	1.7	78
124	Comprehensive Study of the Thermochemistry of First-Row Transition Metal Compounds by Spin Component Scaled MP2 and MP3 Methods. <i>Organometallics</i> , 2004, 23, 5581-5592.	1.1	77
125	The Thermochemistry of London Dispersion-Driven Transition Metal Reactions: Getting the Right Answer for the Right Reason™. <i>ChemistryOpen</i> , 2014, 3, 177-189.	0.9	77
126	Blind Prediction of Binding Affinities for Charged Supramolecular Host-Guest Systems: Achievements and Shortcomings of DFT-D3. <i>Journal of Physical Chemistry B</i> , 2014, 118, 3431-3440.	1.2	77



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127	Excited states using the simplified Tamm-Dancoff-Approach for range-separated hybrid density functionals: development and application. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14408-14419.	1.3	76
128	Assessing Density Functional Theory for Chemically Relevant Open-Shell Transition Metal Reactions. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6134-6151.	2.3	75
129	Structural Importance of Secondary Interactions in Molecules: Origin of Unconventional Conformations of Phosphine-Borane Adducts. <i>Chemistry - A European Journal</i> , 2008, 14, 333-343.	1.7	74
130	Reaction of a Bridged Frustrated Lewis Pair with Nitric Oxide: A Kinetics Study. <i>Journal of the American Chemical Society</i> , 2014, 136, 513-519.	6.6	73
131	Dispersion Corrected Hartree-Fock and Density Functional Theory for Organic Crystal Structure Prediction. <i>Topics in Current Chemistry</i> , 2013, 345, 1-23.	4.0	72
132	Frustrated Lewis Pair-Catalyzed Cycloisomerization of 1,5-Diynes via a <i>endo</i> -dig Cyclization/Protodeborylation Sequence. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 4336-4339.	7.2	72
133	Structure Optimisation of Large Transition-Metal Complexes with Extended Tight-Binding Methods. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 11078-11087.	7.2	72
134	Mechanistic Study of the Titanocene(III)-Catalyzed Radical Arylation of Epoxides. <i>Chemistry - A European Journal</i> , 2015, 21, 280-289.	1.7	71
135	Frustrated Lewis Pair Catalyzed Hydrogenation of Amides: Halides as Active Lewis Base in the Metal-Free Hydrogen Activation. <i>Journal of the American Chemical Society</i> , 2019, 141, 159-162.	6.6	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. <i>Chirality</i> , 2002, 14, 793-797.	1.3	69
137	Titanocene-Catalyzed Radical Opening of N-Acylated Aziridines. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 12654-12657.	7.2	67
138	Enantiomerically Pure Trinuclear Helicates via Diastereoselective Self-Assembly and Characterization of Their Redox Chemistry. <i>Journal of the American Chemical Society</i> , 2014, 136, 11830-11838.	6.6	65
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