Stefan Grimme

List of Publications by Year
in descending order

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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	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
2	HFIPâ€Assisted Single Câ^'F Bond Activation of Trifluoromethyl Ketones using Visibleâ€Light Photoredox Catalysis. Angewandte Chemie, 2022, 134, .	2.0	5
3	HFIPâ€Assisted Single Câ^'F Bond Activation of Trifluoromethyl Ketones using Visibleâ€Light Photoredox Catalysis. Angewandte Chemie - International Edition, 2022, 61, .	13.8	54
4	Increased Antiaromaticity through Pentalene Connection in [n]Cyclo-1,5-dibenzopentalenes. Organic Letters, 2022, 24, 983-988.	4.6	13
5	Frustrated Lewis pair catalyzed hydrodehalogenation of benzyl-halides. Chemical Communications, 2022, 58, 1175-1178.	4.1	11
6	Hydrocarbon Macrocycle Conformer Ensembles and ¹³Câ€NMR Spectra. Angewandte Chemie - International Edition, 2022, 61, .	13.8	10
7	Stereochemical Behavior of Pairs of Pâ€stereogenic Phosphanyl Groups at the Dimethylxanthene Backbone. Chemistry - A European Journal, 2022, , .	3.3	2
8	The long-awaited synthesis and self-assembly of a small rigid C₃-symmetric trilactam. Chemical Communications, 2022, 58, 3751-3754.	4.1	1
9	Benchmark Study on the Calculation of ¹¹⁹Sn NMR Chemical Shifts. Inorganic Chemistry, 2022, 61, 3903-3917.	4.0	11
10	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
11	Dispersion corrected r2SCAN based global hybrid functionals: r2SCANh, r2SCAN0, and r2SCAN50. Journal of Chemical Physics, 2022, 156, 134105.	3.0	32
12	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
13	The Nonâ€Ancillary Nature of Trimethylsilylamide Substituents in Boranes and Borinium Cations. Chemistry - A European Journal, 2022, 28, .	3.3	4
14	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
15	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
16	Computational study of groundâ€state properties of Î¼ ₂ â€bridged group 14 porphyrinic sandwich complexes. Journal of Computational Chemistry, 2022, , .	3.3	1
17	Towards understanding solvation effects on the conformational entropy of non-rigid molecules. Physical Chemistry Chemical Physics, 2022, 24, 12249-12259.	2.8	15
18	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

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19	Catalyst-free CO₂ hydrogenation with BH₃NH₃ in water: DFT mechanistic insights. Physical Chemistry Chemical Physics, 2022, 24, 14159-14164.	2.8	1
20	Conformational Energy Benchmark for Longer n-Alkane Chains. Journal of Physical Chemistry A, 2022, 126, 3521-3535.	2.5	16
21	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, .	3.3	15
22	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
23	Catalytic Isomerization of Unprotected Mesoionic Nâ€Heterocyclic Olefins and Their Lewis Adducts. European Journal of Organic Chemistry, 2022, 2022, .	2.4	3
24	Extended <scp>tightâ€binding</scp> quantum chemistry methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1493.	14.6	596
25	Mechanistic Insights for Dimethyl Sulfoxide Catalyzed Aromatic Chlorination Reactions. ChemCatChem, 2021, 13, 207-211.	3.7	9
26	Quantification of Noncovalent Interactions in Azideâ€“Pnictogen, â€“Chalcogen, and â€“Halogen Contacts. Chemistry - A European Journal, 2021, 27, 4627-4639.	3.3	25
27	Sensory Perception of Nonâ€Deuterated and Deuterated Organic Compounds. Chemistry - A European Journal, 2021, 27, 1046-1056.	3.3	1
28	Theoretical study on conformational energies of transition metal complexes. Physical Chemistry Chemical Physics, 2021, 23, 287-299.	2.8	52
29	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
30	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
31	Comprehensive Benchmark Study on the Calculation of ²⁹Si NMR Chemical Shifts. Inorganic Chemistry, 2021, 60, 272-285.	4.0	14
32	Calculation of absolute molecular entropies and heat capacities made simple. Chemical Science, 2021, 12, 6551-6568.	7.4	83
33	Benchmarking London dispersion corrected density functional theory for noncovalent ionâ€“Ï€ interactions. Physical Chemistry Chemical Physics, 2021, 23, 11635-11648.	2.8	31
34	Lithium Dicyclohexylamide in Transition-Metal-Free Fischerâ€–Tropsch Chemistry. Journal of the American Chemical Society, 2021, 143, 634-638.	13.7	47
35	The power of trichlorosilylation: isolable trisilylated allyl anions, allyl radicals, and allenyl anions. Chemical Science, 2021, 12, 12419-12428.	7.4	4
36	Mechanistic Insights for Nitromethane Activation into Reactive Nitrogenating Reagents. ChemCatChem, 2021, 13, 2132-2137.	3.7	11

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37	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
38	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
39	r2SCAN-3c: A â€œSwiss army knifeâ€•composite electronic-structure method. Journal of Chemical Physics, 2021, 154, 064103.	3.0	290
40	Mechanistic Insights for Acidâ€catalyzed Rearrangement of Quinoxalinâ€2â€one with Diamine and Enamine. ChemCatChem, 2021, 13, 1503-1508.	3.7	5
41	Chiral Dibenzopentaleneâ€Based Conjugated Nanohoops through Stereoselective Synthesis. Angewandte Chemie, 2021, 133, 10775-10784.	2.0	9
42	Chiral Dibenzopentaleneâ€Based Conjugated Nanohoops through Stereoselective Synthesis. Angewandte Chemie - International Edition, 2021, 60, 10680-10689.	13.8	29
43	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
44	Perspective on Simplified Quantum Chemistry Methods for Excited States and Response Properties. Journal of Physical Chemistry A, 2021, 125, 3841-3851.	2.5	15
45	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
46	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
47	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
48	Titanoceneâ€Catalyzed [2+2] Cycloaddition of Bisenones and Comparison with Photoredox Catalysis and Established Methods. Angewandte Chemie, 2021, 133, 14460-14465.	2.0	4
49	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
50	Efficient Quantum-Chemical Calculations of Acid Dissociation Constants from Free-Energy Relationships. Journal of Physical Chemistry A, 2021, 125, 5681-5692.	2.5	18
51	LiAlH 4 â€catalyzed Imine Hydrogenation with Dihydrogen: New DFT Mechanistic Insights. ChemCatChem, 2021, 13, 3401-3404.	3.7	9
52	Robust and Efficient Implicit Solvation Model for Fast Semiempirical Methods. Journal of Chemical Theory and Computation, 2021, 17, 4250-4261.	5.3	186
53	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
54	Facile Synthesis of Cyanide and Isocyanides from CO. Angewandte Chemie, 2021, 133, 17102-17106.	2.0	4

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55	Facile Synthesis of Cyanide and Isocyanides from CO. Angewandte Chemie - International Edition, 2021, 60, 16965-16969.	13.8	15
56	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
57	Revisiting conformations of methyl lactate in water and methanol. Journal of Chemical Physics, 2021, 155, 024507.	3.0	16
58	[Cl@Si₂₀H₂₀]^{â^'}: Parent Siladodecahedrane with Endohedral Chloride Ion. Journal of the American Chemical Society, 2021, 143, 10865-10871.	13.7	20
59	High-Throughput Non-targeted Chemical Structure Identification Using Gas-Phase Infrared Spectra. Analytical Chemistry, 2021, 93, 10688-10696.	6.5	4
60	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
61	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
62	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
63	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
64	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
65	Steric Influence on Reactions of Benzyl Potassium Species with CO. Chemistry - an Asian Journal, 2021, 16, 3640-3644.	3.3	7
66	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
67	Synthesis and Mechanistic Insights of the Formation of 3-Hydroxyquinolin-2-ones including Viridicatin from 2-Chloro-N,3-diaryloxirane-2-carboxamides under Acid-Catalyzed Rearrangements. Journal of Organic Chemistry, 2021, 86, 13514-13534.	3.2	7
68	Hydrogenation of Secondary Amides using Phosphane Oxide and Frustrated Lewis Pair Catalysis. Chemistry - A European Journal, 2021, 27, 14179-14183.	3.3	9
69	Nanopatterns of molecular spoked wheels as giant homologues of benzene tricarboxylic acids. Chemical Science, 2021, 12, 9352-9358.	7.4	7
70	Hydrogen atom transfer rates from Tp-containing metal-hydrides to trityl radicals. Canadian Journal of Chemistry, 2021, 99, 216-220.	1.1	5
71	Selective Catalytic Frustrated Lewis Pair Hydrogenation of CO₂ in the Presence of Silylhalides. Angewandte Chemie - International Edition, 2021, 60, 25771-25775.	13.8	26
72	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

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73	Selective catalytic Frustrated Lewis Pair Hydrogenation of CO2 in the Presence of Silylhalides. Angewandte Chemie, 2021, 133, 25975.	2.0	7
74	Automated Quantum Chemistry-Based Calculation of Optical Rotation for Large Flexible Molecules. Journal of Organic Chemistry, 2021, 86, 15522-15531.	3.2	18
75	Boron-Catalyzed Hydroarylation of 1,3-Dienes with Arylamines. Organic Letters, 2021, 23, 8952-8957.	4.6	13
76	Ligand Protonation at Carbon, not Nitrogen, during H₂ Production with Amine-Rich Iron Electrocatalysts. Inorganic Chemistry, 2021, 60, 17407-17413.	4.0	6
77	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
78	Nanoscale Ï€-conjugated ladders. Nature Communications, 2021, 12, 6614.	12.8	8
79	Quickstart guide to model structures and interactions of artificial molecular muscles with efficient computational methods. Chemical Communications, 2021, 58, 258-261.	4.1	3
80	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
81	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
82	Heterobifunctional Rotaxanes for Asymmetric Catalysis. Angewandte Chemie, 2020, 132, 5140-5145.	2.0	18
83	Heterobifunctional Rotaxanes for Asymmetric Catalysis. Angewandte Chemie - International Edition, 2020, 59, 5102-5107.	13.8	56
84	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
85	Mechanistic Insights for Anilineâ€Catalyzed Halogenation Reactions. ChemCatChem, 2020, 12, 5369-5373.	3.7	5
86	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
87	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
88	Benchmark Study of Electrochemical Redox Potentials Calculated with Semiempirical and DFT Methods. Journal of Physical Chemistry A, 2020, 124, 7166-7176.	2.5	45
89	Efficient Computation of Free Energy Contributions for Association Reactions of Large Molecules. Journal of Physical Chemistry Letters, 2020, 11, 6606-6611.	4.6	49
90	Modeling of spinâ€“spin distance distributions for nitroxide labeled biomacromolecules. Physical Chemistry Chemical Physics, 2020, 22, 24282-24290.	2.8	32

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91	Mechanistic Insights for Iodane Mediated Aromatic Halogenation Reactions. ChemCatChem, 2020, 12, 6186-6190.	3.7	5
92	Simplified time-dependent density functional theory (sTD-DFT) for molecular optical rotation. Journal of Chemical Physics, 2020, 153, 084116.	3.0	25
93	Robust Atomistic Modeling of Materials, Organometallic, and Biochemical Systems. Angewandte Chemie, 2020, 132, 15795-15803.	2.0	40
94	The first microsolvation step for furans: New experiments and benchmarking strategies. Journal of Chemical Physics, 2020, 152, 164303.	3.0	28
95	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
96	BNB-Doped Phenalenyls: Modular Synthesis, Optoelectronic Properties, and One-Electron Reduction. Journal of the American Chemical Society, 2020, 142, 11072-11083.	13.7	63
97	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
98	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
99	Extension and evaluation of the D4 London-dispersion model for periodic systems. Physical Chemistry Chemical Physics, 2020, 22, 8499-8512.	2.8	138
100	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
101	Acidâ€Catalyzed Rearrangements of 3â€Aryloxiraneâ€2â€Carboxamides: Novel DFT Mechanistic Insights. ChemistryOpen, 2020, 9, 743-747.	1.9	10
102	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
103	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
104	Quantum Chemical Calculation of Molecular and Periodic Peptide and Protein Structures. Journal of Physical Chemistry B, 2020, 124, 3636-3646.	2.6	33
105	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
106	Robust Atomistic Modeling of Materials, Organometallic, and Biochemical Systems. Angewandte Chemie - International Edition, 2020, 59, 15665-15673.	13.8	224
107	Frustrated Lewis Pair Catalyzed Reduction of Carbon Dioxide Using Hydroboranes: New DFT Mechanistic Insights. ChemCatChem, 2020, 12, 3656-3660.	3.7	14
108	Automated exploration of the low-energy chemical space with fast quantum chemical methods. Physical Chemistry Chemical Physics, 2020, 22, 7169-7192.	2.8	966

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109	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
110	Extension of the element parameter set for ultra-fast excitation spectra calculation (sTDA-xTB). Molecular Physics, 2019, 117, 1104-1116.	1.7	4
111	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
112	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
113	Acylation Reactions of Dibenzoâ€7â€phosphanorbornadiene: DFT Mechanistic Insights. ChemistryOpen, 2019, 8, 807-810.	1.9	9
114	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.	2.5	5
115	Thermodynamics of H⁺/H^{â€¢}/H^{â€“}/e^{â€“} Transfer from [CpV(CO)₃H]^{â^'}: Comparisons to the Isoelectronic CpCr(CO)₃H. Organometallics, 2019, 38, 4319-4328.	2.3	10
116	Boron Lewis Acid-Catalyzed Regioselective Hydrothiolation of Conjugated Dienes with Thiols. ACS Catalysis, 2019, 9, 11627-11633.	11.2	25
117	Catalytic Difunctionalization of Unactivated Alkenes with Unreactive Hexamethyldisilane through Regeneration of Silylium Ions. Angewandte Chemie - International Edition, 2019, 58, 17307-17311.	13.8	26
118	Katalytische Difunktionalisierung von nichtaktivierten Alkenen mit reaktionstrÃgem Hexamethyldisilan durch Neubildung von Silyliumionen. Angewandte Chemie, 2019, 131, 17468-17472.	2.0	5
119	Calculation of Electron Ionization Mass Spectra with Semiempirical GFNn-xTB Methods. ACS Omega, 2019, 4, 15120-15133.	3.5	33
120	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
121	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
122	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
123	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
124	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
125	Structure Optimisation of Large Transitionâ€Metal Complexes with Extended Tightâ€Binding Methods. Angewandte Chemie - International Edition, 2019, 58, 11078-11087.	13.8	72
126	Structure Optimisation of Large Transitionâ€Metal Complexes with Extended Tightâ€Binding Methods. Angewandte Chemie, 2019, 131, 11195-11204.	2.0	21

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127	Structural and Conformational Studies on Carboxamides of 5,6-Diaminouracilsâ€"Precursors of Biologically Active Xanthine Derivatives. Molecules, 2019, 24, 2168.	3.8	2
128	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
129	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
130	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
131	A generally applicable atomic-charge dependent London dispersion correction. Journal of Chemical Physics, 2019, 150, 154122.	3.0	697
132	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
133	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
134	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
135	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
136	The Chiral Trimer and a Metastable Chiral Dimer of Achiral Hexafluoroisopropanol: A Multiâ€Messenger Study. Angewandte Chemie, 2019, 131, 5134-5138.	2.0	20
137	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
138	Reduction of Phosphine Oxide by Using Chlorination Reagents and Dihydrogen: DFT Mechanistic Insights. Chemistry - A European Journal, 2019, 25, 4670-4672.	3.3	16
139	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
140	Understanding and Quantifying London Dispersion Effects in Organometallic Complexes. Accounts of Chemical Research, 2019, 52, 258-266.	15.6	117
141	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
142	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
143	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
144	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

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145	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
146	Solid state frustrated Lewis pair chemistry. Chemical Science, 2018, 9, 4859-4865.	7.4	35
147	B97-3c: A revised low-cost variant of the B97-D density functional method. Journal of Chemical Physics, 2018, 148, 064104.	3.0	400
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