Stefan Grimme

List of Publications by Year in Descending Order

342 papers	92,457 citations	89 h-index	303 g-index
375 ext. papers	109,789 ext. citations	7.2 avg, IF	9.27 L-index

#	Paper	IF	Citations
342	The long-awaited synthesis and self-assembly of a small rigid -symmetric trilactam.. *Chemical Communications*, **2022**,	5.8	1
341	Benchmark Study on the Calculation of Sn NMR Chemical Shifts.. *Inorganic Chemistry*, **2022**, 61, 3903-3917	5.1	1
340	Dispersion corrected rSCAN based global hybrid functionals: rSCANh, rSCAN0, and rSCAN50.. *Journal of Chemical Physics*, **2022**, 156, 134105	3.9	4
339	Hydrogen atom transfer rates from Tp-containing metal-hydrides to trityl radicals. *Canadian Journal of Chemistry*, **2021**, 99, 216-220	0.9	1
338	Ligand Protonation at Carbon, not Nitrogen, during H Production with Amine-Rich Iron Electrocatalysts. *Inorganic Chemistry*, **2021**, 60, 17407-17413	5.1	0
337	Nanoscale □conjugated ladders. *Nature Communications*, **2021**, 12, 6614	17.4	2
336	Computer-aided simulation of infrared spectra of ethanol conformations in gas, liquid and in CCl solution. *Journal of Computational Chemistry*, **2021**,	3.5	4
335	HFIP-Assisted Single C-F Bond Activation of Trifluoromethyl Ketones using Visible-Light Photoredox Catalysis. *Angewandte Chemie - International Edition*, **2021**,	16.4	8
334	Selective Catalytic Frustrated Lewis Pair Hydrogenation of CO in the Presence of Silylhalides. *Angewandte Chemie - International Edition*, **2021**, 60, 25771-25775	16.4	2
333	Selective Catalytic Frustrated Lewis Pair Hydrogenation of CO2 in the Presence of Silylhalides. *Angewandte Chemie*, **2021**, 133, 25975	3.6	1
332	Automated Quantum Chemistry-Based Calculation of Optical Rotation for Large Flexible Molecules. *Journal of Organic Chemistry*, **2021**, 86, 15522-15531	4.2	3
331	Boron-Catalyzed Hydroarylation of 1,3-Dienes with Arylamines. *Organic Letters*, **2021**, 23, 8952-8957	6.2	3
330	Chiral Dibenzopentalene-Based Conjugated Nanohoops through Stereoselective Synthesis. *Angewandte Chemie*, **2021**, 133, 10775-10784	3.6	1
329	Chiral Dibenzopentalene-Based Conjugated Nanohoops through Stereoselective Synthesis. *Angewandte Chemie - International Edition*, **2021**, 60, 10680-10689	16.4	9
328	Efficient Quantum Chemical Calculation of Structure Ensembles and Free Energies for Nonrigid Molecules. *Journal of Physical Chemistry A*, **2021**, 125, 4039-4054	2.8	32
327	Perspective on Simplified Quantum Chemistry Methods for Excited States and Response Properties. *Journal of Physical Chemistry A*, **2021**, 125, 3841-3851	2.8	5
326	Comment on □he Nature of Chalcogen-Bonding-Type Tellurium□Nitrogen Interactions□Fixing the Description of Finite-Temperature Effects Restores the Agreement Between Experiment and Theory. *Angewandte Chemie*, **2021**, 133, 13252-13257	3.6	2

325	Titanocene-Catalyzed [2+2] Cycloaddition of Bisenones and Comparison with Photoredox Catalysis and Established Methods. *Angewandte Chemie - International Edition*, **2021**, 60, 14339-14344	16.4	4
324	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	3.5	4
323	Titanocene-Catalyzed [2+2] Cycloaddition of Bisenones and Comparison with Photoredox Catalysis and Established Methods. *Angewandte Chemie*, **2021**, 133, 14460-14465	3.6	1
322	Comment on "The Nature of Chalcogen-Bonding-Type Tellurium-Nitrogen Interactions": Fixing the Description of Finite-Temperature Effects Restores the Agreement Between Experiment and Theory. *Angewandte Chemie - International Edition*, **2021**, 60, 13144-13149	16.4	4
321	Efficient Quantum-Chemical Calculations of Acid Dissociation Constants from Free-Energy Relationships. *Journal of Physical Chemistry A*, **2021**, 125, 5681-5692	2.8	5
320	LiAlH4-catalyzed Imine Hydrogenation with Dihydrogen: New DFT Mechanistic Insights. *ChemCatChem*, **2021**, 13, 3401-3404	5.2	2
319	Robust and Efficient Implicit Solvation Model for Fast Semiempirical Methods. *Journal of Chemical Theory and Computation*, **2021**, 17, 4250-4261	6.4	31
318	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	3.5	7
317	Facile Synthesis of Cyanide and Isocyanides from CO. *Angewandte Chemie*, **2021**, 133, 17102-17106	3.6	2
316	Facile Synthesis of Cyanide and Isocyanides from CO. *Angewandte Chemie - International Edition*, **2021**, 60, 16965-16969	16.4	4
315	Frustrated Lewis-Pair Neighbors at the Xanthene Framework: Epimerization at Phosphorus and Cooperative Formation of Macrocyclic Adduct Structures. *Chemistry - A European Journal*, **2021**, 27, 12104-12114	4.8	0
314	Revisiting conformations of methyl lactate in water and methanol. *Journal of Chemical Physics*, **2021**, 155, 024507	3.9	6
313	[Cl@SiH]: Parent Siladodecahedrane with Endohedral Chloride Ion. *Journal of the American Chemical Society*, **2021**, 143, 10865-10871	16.4	4
312	Extended tight-binding quantum chemistry methods. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1493	7.9	149
311	Mechanistic Insights for Dimethyl Sulfoxide Catalyzed Aromatic Chlorination Reactions. *ChemCatChem*, **2021**, 13, 207-211	5.2	2
310	Quantification of Noncovalent Interactions in Azide-Pnictogen, -Chalcogen, and -Halogen Contacts. *Chemistry - A European Journal*, **2021**, 27, 4627-4639	4.8	11
309	Sensory Perception of Non-Deuterated and Deuterated Organic Compounds. *Chemistry - A European Journal*, **2021**, 27, 1046-1056	4.8	1
308	Theoretical study on conformational energies of transition metal complexes. *Physical Chemistry Chemical Physics*, **2021**, 23, 287-299	3.6	24

307	Oxidation Under Reductive Conditions: From Benzylic Ethers to Acetals with Perfect Atom-Economy by Titanocene(III) Catalysis. *Angewandte Chemie - International Edition*, **2021**, 60, 5482-5488	16.4	8
306	Oxidation Under Reductive Conditions: From Benzylic Ethers to Acetals with Perfect Atom-Economy by Titanocene(III) Catalysis. *Angewandte Chemie*, **2021**, 133, 5542-5548	3.6	5
305	Comprehensive Benchmark Study on the Calculation of Si NMR Chemical Shifts. *Inorganic Chemistry*, **2021**, 60, 272-285	5.1	9
304	Calculation of absolute molecular entropies and heat capacities made simple. *Chemical Science*, **2021**, 12, 6551-6568	9.4	17
303	Benchmarking London dispersion corrected density functional theory for noncovalent ion-π interactions. *Physical Chemistry Chemical Physics*, **2021**, 23, 11635-11648	3.6	7
302	Lithium Dicyclohexylamide in Transition-Metal-Free Fischer-Tropsch Chemistry. *Journal of the American Chemical Society*, **2021**, 143, 634-638	16.4	22
301	The power of trichlorosilylation: isolable trisilylated allyl anions, allyl radicals, and allenyl anions. *Chemical Science*, **2021**, 12, 12419-12428	9.4	0
300	Mechanistic Insights for Nitromethane Activation into Reactive Nitrogenating Reagents. *ChemCatChem*, **2021**, 13, 2132-2137	5.2	2
299	Ox-SLIM: Synthesis of and Site-Specific Labelling with a Highly Hydrophilic Trityl Spin Label. *Chemistry - A European Journal*, **2021**, 27, 5292-5297	4.8	13
298	Single-Point Hessian Calculations for Improved Vibrational Frequencies and Rigid-Rotor-Harmonic-Oscillator Thermodynamics. *Journal of Chemical Theory and Computation*, **2021**, 17, 1701-1714	6.4	20
297	rSCAN-3c: A "Swiss army knife" composite electronic-structure method. *Journal of Chemical Physics*, **2021**, 154, 064103	3.9	65
296	Mechanistic Insights for Acid-catalyzed Rearrangement of Quinoxalin-2-one with Diamine and Enamine. *ChemCatChem*, **2021**, 13, 1503-1508	5.2	2
295	High-Throughput Non-targeted Chemical Structure Identification Using Gas-Phase Infrared Spectra. *Analytical Chemistry*, **2021**, 93, 10688-10696	7.8	
294	PCM-ROKS for the Description of Charge-Transfer States in Solution: Singlet-Triplet Gaps with Chemical Accuracy from Open-Shell Kohn-Sham Reaction-Field Calculations. *Journal of Physical Chemistry Letters*, **2021**, 12, 8470-8480	6.4	7
293	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	3.9	1
292	Reactions of a Dilithiomethane with CO and N O: An Avenue to an Anionic Ketene and a Hexafunctionalized Benzene. *Angewandte Chemie - International Edition*, **2021**, 60, 25281-25285	16.4	4
291	Assessing Density Functional Theory for Chemically Relevant Open-Shell Transition Metal Reactions. *Journal of Chemical Theory and Computation*, **2021**, 17, 6134-6151	6.4	19
290	Steric Influence on Reactions of Benzyl Potassium Species with CO. *Chemistry - an Asian Journal*, **2021**, 16, 3640-3644	4.5	1

289	All-Atom Quantum Mechanical Calculation of the Second-Harmonic Generation of Fluorescent Proteins. *Journal of Physical Chemistry Letters*, **2021**, 12, 9684-9690	6.4	2
288	Synthesis and Mechanistic Insights of the Formation of 3-Hydroxyquinolin-2-ones including Viridicatin from 2-Chloro-,3-diaryloxirane-2-carboxamides under Acid-Catalyzed Rearrangements. *Journal of Organic Chemistry*, **2021**, 86, 13514-13534	4.2	2
287	Hydrogenation of Secondary Amides using Phosphane Oxide and Frustrated Lewis Pair Catalysis. *Chemistry - A European Journal*, **2021**, 27, 14179-14183	4.8	5
286	Nanopatterns of molecular spoked wheels as giant homologues of benzene tricarboxylic acids. *Chemical Science*, **2021**, 12, 9352-9358	9.4	3
285	Quantum Chemical Calculation and Evaluation of Partition Coefficients for Classical and Emerging Environmentally Relevant Organic Compounds.. *Environmental Science & Technology*, **2021**,	10.3	2
284	Designing a Solution-Stable Distannene: The Decisive Role of London Dispersion Effects in the Structure and Properties of {Sn(CH-2,4,6-Cy)} (Cy = Cyclohexyl).. *Journal of the American Chemical Society*, **2021**, 143, 21478-21483	16.4	2
283	Robust Atomistic Modeling of Materials, Organometallic, and Biochemical Systems. *Angewandte Chemie*, **2020**, 132, 15795-15803	3.6	20
282	The first microsolvation step for furans: New experiments and benchmarking strategies. *Journal of Chemical Physics*, **2020**, 152, 164303	3.9	14
281	Building up Strain in One Step: Synthesis of an Edge-Fused Double Silacyclobutene from an Extensively Trichlorosilylated Butadiene Dianion. *Angewandte Chemie - International Edition*, **2020**, 59, 16181-16187	16.4	3
280	BNB-Doped Phenalenyls: Modular Synthesis, Optoelectronic Properties, and One-Electron Reduction. *Journal of the American Chemical Society*, **2020**, 142, 11072-11083	16.4	28
279	Building up Strain in One Step: Synthesis of an Edge-Fused Double Silacyclobutene from an Extensively Trichlorosilylated Butadiene Dianion. *Angewandte Chemie*, **2020**, 132, 16315-16321	3.6	1
278	Dynamic Structural Effects on the Second-Harmonic Generation of Tryptophane-Rich Peptides and Gramicidin A. *Journal of Physical Chemistry B*, **2020**, 124, 2568-2578	3.4	8
277	Extension and evaluation of the D4 London-dispersion model for periodic systems. *Physical Chemistry Chemical Physics*, **2020**, 22, 8499-8512	3.6	42
276	What is the role of acid-acid interactions in asymmetric phosphoric acid organocatalysis? A detailed mechanistic study using interlocked and non-interlocked catalysts. *Chemical Science*, **2020**, 11, 4381-4390	8.4	20
275	Acid-Catalyzed Rearrangements of 3-Aryloxirane-2-Carboxamides: Novel DFT Mechanistic Insights. *ChemistryOpen*, **2020**, 9, 743-747	2.3	2
274	Fast and Accurate Quantum Chemical Modeling of Infrared Spectra of Condensed-Phase Systems. *Journal of Physical Chemistry B*, **2020**, 124, 6664-6670	3.4	10
273	Semiautomated Transition State Localization for Organometallic Complexes with Semiempirical Quantum Chemical Methods. *Journal of Chemical Theory and Computation*, **2020**, 16, 2002-2012	6.4	32
272	Quantum Chemical Calculation of Molecular and Periodic Peptide and Protein Structures. *Journal of Physical Chemistry B*, **2020**, 124, 3636-3646	3.4	17

271	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	16.4	39
270	Robust Atomistic Modeling of Materials, Organometallic, and Biochemical Systems. *Angewandte Chemie - International Edition*, **2020**, 59, 15665-15673	16.4	93
269	Automated exploration of the low-energy chemical space with fast quantum chemical methods. *Physical Chemistry Chemical Physics*, **2020**, 22, 7169-7192	3.6	327
268	Influencing the Self-Sorting Behavior of [2.2]Paracyclophane-Based Ligands by Introducing Isostructural Binding Motifs. *Chemistry - A European Journal*, **2020**, 26, 3335-3347	4.8	9
267	Heterobifunctional Rotaxanes for Asymmetric Catalysis. *Angewandte Chemie*, **2020**, 132, 5140-5145	3.6	9
266	Heterobifunctional Rotaxanes for Asymmetric Catalysis. *Angewandte Chemie - International Edition*, **2020**, 59, 5102-5107	16.4	28
265	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	6.4	12
264	Mechanistic Insights for Aniline-Catalyzed Halogenation Reactions. *ChemCatChem*, **2020**, 12, 5369-5373	5.2	1
263	Efficient Calculation of Small Molecule Binding in Metal Organic Frameworks and Porous Organic Cages. *Journal of Physical Chemistry C*, **2020**, 124, 27529-27541	3.8	13
262	A Unified Strategy for the Chemically Intuitive Interpretation of Molecular Optical Response Properties. *Journal of Chemical Theory and Computation*, **2020**, 16, 7709-7720	6.4	5
261	Benchmark Study of Electrochemical Redox Potentials Calculated with Semiempirical and DFT Methods. *Journal of Physical Chemistry A*, **2020**, 124, 7166-7176	2.8	15
260	Efficient Computation of Free Energy Contributions for Association Reactions of Large Molecules. *Journal of Physical Chemistry Letters*, **2020**, 11, 6606-6611	6.4	27
259	Modeling of spin-spin distance distributions for nitroxide labeled biomacromolecules. *Physical Chemistry Chemical Physics*, **2020**, 22, 24282-24290	3.6	16
258	Mechanistic Insights for Iodane Mediated Aromatic Halogenation Reactions. *ChemCatChem*, **2020**, 12, 6186-6190	5.2	1
257	Simplified time-dependent density functional theory (sTD-DFT) for molecular optical rotation. *Journal of Chemical Physics*, **2020**, 153, 084116	3.9	10
256	Frustrated Lewis Pair Catalyzed Reduction of Carbon Dioxide Using Hydroboranes: New DFT Mechanistic Insights. *ChemCatChem*, **2020**, 12, 3656-3660	5.2	6
255	Katalytische Difunktionalisierung von nichtaktivierten Alkenen mit reaktionsträgem Hexamethyldisilan durch Neubildung von Silyliumionen. *Angewandte Chemie*, **2019**, 131, 17468-17472	3.6	5
254	Calculation of Electron Ionization Mass Spectra with Semiempirical GFNn-xTB Methods. *ACS Omega*, **2019**, 4, 15120-15133	3.9	17

253	Folding of unstructured peptoids and formation of hetero-bimetallic peptoid complexes upon side-chain-to-metal coordination. *Chemical Science*, **2019**, 10, 620-632	9.4	18
252	Synthesis of μ-Oxo-Bridged Iron(III) Tetraphenylporphyrin-Spacer-Nitroxide Dimers and their Structural and Dynamics Characterization by using EPR and MD Simulations. *Chemistry - A European Journal*, **2019**, 25, 2586-2596	4.8	9
251	TEMPO-Mediated Catalysis of the Sterically Hindered Hydrogen Atom Transfer Reaction between (CPh)Cr(CO)H and a Trityl Radical. *Journal of the American Chemical Society*, **2019**, 141, 1882-1886	16.4	16
250	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	3.6	17
249	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	2.8	9
248	Structure Optimisation of Large Transition-Metal Complexes with Extended Tight-Binding Methods. *Angewandte Chemie - International Edition*, **2019**, 58, 11078-11087	16.4	38
247	Structure Optimisation of Large Transition-Metal Complexes with Extended Tight-Binding Methods. *Angewandte Chemie*, **2019**, 131, 11195-11204	3.6	13
246	Structural and Conformational Studies on Carboxamides of 5,6-Diaminouracils-Precursors of Biologically Active Xanthine Derivatives. *Molecules*, **2019**, 24,	4.8	1
245	Borane-Catalyzed Hydrogenation of Tertiary Amides Activated by Oxalyl Chloride: DFT Mechanistic Insights. *European Journal of Organic Chemistry*, **2019**, 2019, 4609-4612	3.2	5
244	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	3.6	15
243	Pulsed EPR Dipolar Spectroscopy under the Breakdown of the High-Field Approximation: The High-Spin Iron(III) Case. *Chemistry - A European Journal*, **2019**, 25, 8820-8828	4.8	8
242	A generally applicable atomic-charge dependent London dispersion correction. *Journal of Chemical Physics*, **2019**, 150, 154122	3.9	300
241	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	3.2	6
240	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	3.9	15
239	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	2.8	13
238	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	6.4	240
237	The Chiral Trimer and a Metastable Chiral Dimer of Achiral Hexafluoroisopropanol: A Multi-Messenger Study. *Angewandte Chemie*, **2019**, 131, 5134-5138	3.6	15
236	GFN2-xTB-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	6.4	717

235	Extension of the element parameter set for ultra-fast excitation spectra calculation (sTDA-xTB). *Molecular Physics*, **2019**, 117, 1104-1116	1.7	3
234	Isolation and Computational Studies of a Series of Terphenyl Substituted Diplumbynes with Ligand Dependent Lead-Lead Multiple-Bonding Character. *Journal of the American Chemical Society*, **2019**, 141, 14370-14383	16.4	12
233	Pulsed EPR Dipolar Spectroscopy on Spin Pairs with one Highly Anisotropic Spin Center: The Low-Spin Fe Case. *Chemistry - A European Journal*, **2019**, 25, 14388-14398	4.8	14
232	Acylation Reactions of Dibenzo-7-phosphanorbornadiene: DFT Mechanistic Insights. *ChemistryOpen* , **2019**, 8, 807-810	2.3	5
231	Are Fully Conjugated Expanded Indenofluorenes Analogues and Diindeno[]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	2.8	5
230	Thermodynamics of H+/H□H/e□Transfer from [CpV(CO)3H]□Comparisons to the Isoelectronic CpCr(CO)3H. *Organometallics*, **2019**, 38, 4319-4328	3.8	7
229	Boron Lewis Acid-Catalyzed Regioselective Hydrothiolation of Conjugated Dienes with Thiols. *ACS Catalysis*, **2019**, 9, 11627-11633	13.1	11
228	Catalytic Difunctionalization of Unactivated Alkenes with Unreactive Hexamethyldisilane through Regeneration of Silylium Ions. *Angewandte Chemie - International Edition*, **2019**, 58, 17307-17311	16.4	18
227	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	0.9	8
226	Reduction of Phosphine Oxide by Using Chlorination Reagents and Dihydrogen: DFT Mechanistic Insights. *Chemistry - A European Journal*, **2019**, 25, 4670-4672	4.8	11
225	The Chiral Trimer and a Metastable Chiral Dimer of Achiral Hexafluoroisopropanol: A Multi-Messenger Study. *Angewandte Chemie - International Edition*, **2019**, 58, 5080-5084	16.4	30
224	Understanding and Quantifying London Dispersion Effects in Organometallic Complexes. *Accounts of Chemical Research*, **2019**, 52, 258-266	24.3	69
223	Aggregation Behavior of a Six-Membered Cyclic Frustrated Phosphane/Borane Lewis Pair: Formation of a Supramolecular Cyclooctameric Macrocyclic Ring System. *Angewandte Chemie - International Edition*, **2019**, 58, 882-886	16.4	20
222	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	16.4	44
221	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	3.9	23
220	Donor-acceptor interactions between cyclic trinuclear pyridinate gold(i)-complexes and electron-poor guests: nature and energetics of guest-binding and templating on graphite. *Chemical Science*, **2018**, 9, 3477-3483	9.4	15
219	Solid state frustrated Lewis pair chemistry. *Chemical Science*, **2018**, 9, 4859-4865	9.4	24
218	B97-3c: A revised low-cost variant of the B97-D density functional method. *Journal of Chemical Physics*, **2018**, 148, 064104	3.9	221

217	The furan microsolvation blind challenge for quantum chemical methods: First steps. *Journal of Chemical Physics*, **2018**, 148, 014301	3.9	34
216	Bismuth as a versatile cation for luminescence in coordination polymers from BiX/4,4′-bipy: understanding of photophysics by quantum chemical calculations and structural parallels to lanthanides. *Dalton Transactions*, **2018**, 47, 7669-7681	4.3	35
215	Comprehensive Thermochemical Benchmark Set of Realistic Closed-Shell Metal Organic Reactions. *Journal of Chemical Theory and Computation*, **2018**, 14, 2596-2608	6.4	122
214	Counterintuitive Interligand Angles in the Diaryls E{C6H3-2,6-(C6H2-2,4,6-iPr3)2}2 (E = Ge, Sn, or Pb) and Related Species: The Role of London Dispersion Forces. *Organometallics*, **2018**, 37, 2075-2085	3.8	18
213	Exhaustively Trichlorosilylated C and C Building Blocks: Beyond the M□ller-Rochow Direct Process. *Journal of the American Chemical Society*, **2018**, 140, 9696-9708	16.4	12
212	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	3.9	28
211	Elektrophile Formylierung von Aromaten durch silyliumionvermittelte Aktivierung von Kohlenmonoxid. *Angewandte Chemie*, **2018**, 130, 8433-8437	3.6	11
210	Electrophilic Formylation of Arenes by Silylium Ion Mediated Activation of Carbon Monoxide. *Angewandte Chemie - International Edition*, **2018**, 57, 8301-8305	16.4	28
209	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	4.2	31
208	Synthesis of 1,3-Amino Alcohols by Hydroxy-Directed Aziridination and Aziridine Hydrosilylation. *Angewandte Chemie*, **2018**, 130, 13716-13720	3.6	3
207	Synthesis of 1,3-Amino Alcohols by Hydroxy-Directed Aziridination and Aziridine Hydrosilylation. *Angewandte Chemie - International Edition*, **2018**, 57, 13528-13532	16.4	13
206	Formation of macrocyclic ring systems by carbonylation of trifunctional P/B/B frustrated Lewis pairs. *Chemical Science*, **2018**, 9, 1544-1550	9.4	25
205	Computerchemie: das Schicksal aktueller Methoden und zuk□ftige Herausforderungen. *Angewandte Chemie*, **2018**, 130, 4241-4248	3.6	9
204	Computational Chemistry: The Fate of Current Methods and Future Challenges. *Angewandte Chemie - International Edition*, **2018**, 57, 4170-4176	16.4	85
203	Raising the Bar in Aromatic Donor-Acceptor Interactions with Cyclic Trinuclear Gold(I) Complexes as Strong □Donors. *Journal of the American Chemical Society*, **2018**, 140, 17932-17944	16.4	29
202	Aggregation Behavior of a Six-Membered Cyclic Frustrated Phosphane/Borane Lewis Pair: Formation of a Supramolecular Cyclooctameric Macrocyclic Ring System. *Angewandte Chemie*, **2018**, 131, 892	3.6	
201	Reduktion von Phosphanoxiden mit Oxalylchlorid und Wasserstoff, vermittelt durch ein elektrophiles Phosphoniumkation. *Angewandte Chemie*, **2018**, 130, 15473-15476	3.6	4
200	Electrophilic Phosphonium Cation-Mediated Phosphane Oxide Reduction Using Oxalyl Chloride and Hydrogen. *Angewandte Chemie - International Edition*, **2018**, 57, 15253-15256	16.4	20

199	Borane-Catalyzed Synthesis of Quinolines Bearing Tetrasubstituted Stereocenters by Hydride Abstraction-Induced Electrocyclization. *Chemistry - A European Journal*, **2018**, 24, 16287-16291	4.8	35
198	Towards full Quantum-Mechanics-based Protein-Ligand Binding Affinities. *ChemPhysChem*, **2017**, 18, 898-905	3.2	35
197	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	16.4	39
196	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 = 1-86). *Journal of Chemical Theory and Computation*, **2017**, 13, 1989-2009	6.4	592
195	London Dispersion Enables the Shortest Intermolecular Hydrocarbon H H Contact. *Journal of the American Chemical Society*, **2017**, 139, 7428-7431	16.4	85
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List of Publications