Stefan Grimme

List of Publications by Citations

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	A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *Journal of Chemical Physics*, **2010**, 132, 154104	3.9	23773
341	Semiempirical GGA-type density functional constructed with a long-range dispersion correction. *Journal of Computational Chemistry*, **2006**, 27, 1787-99	3.5	19063
340	Effect of the damping function in dispersion corrected density functional theory. *Journal of Computational Chemistry*, **2011**, 32, 1456-65	3.5	10429
339	Accurate description of van der Waals complexes by density functional theory including empirical corrections. *Journal of Computational Chemistry*, **2004**, 25, 1463-73	3.5	3746
338	Semiempirical hybrid density functional with perturbative second-order correlation. *Journal of Chemical Physics*, **2006**, 124, 034108	3.9	2321
337	Density functional theory with London dispersion corrections. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 211-228	7.9	1645
336	Improved second-order M□ller-Plesset perturbation theory by separate scaling of parallel- and antiparallel-spin pair correlation energies. *Journal of Chemical Physics*, **2003**, 118, 9095-9102	3.9	1471
335	A thorough benchmark of density functional methods for general main group thermochemistry, kinetics, and noncovalent interactions. *Physical Chemistry Chemical Physics*, **2011**, 13, 6670-88	3.6	1347
334	Supramolecular binding thermodynamics by dispersion-corrected density functional theory. *Chemistry - A European Journal*, **2012**, 18, 9955-64	4.8	974
333	Double-hybrid density functionals with long-range dispersion corrections: higher accuracy and extended applicability. *Physical Chemistry Chemical Physics*, **2007**, 9, 3397-406	3.6	890
332	Efficient and Accurate Double-Hybrid-Meta-GGA Density Functionals-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	6.4	841
331	Do special noncovalent pi-pi stacking interactions really exist?. *Angewandte Chemie - International Edition*, **2008**, 47, 3430-4	16.4	808
330	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	3.6	738
329	Dispersion-Corrected Mean-Field Electronic Structure Methods. *Chemical Reviews*, **2016**, 116, 5105-54	68.1	738
328	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
327	Density functional theory with dispersion corrections for supramolecular structures, aggregates, and complexes of (bio)organic molecules. *Organic and Biomolecular Chemistry*, **2007**, 5, 741-58	3.9	636
326	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

325	Reversible metal-free carbon dioxide binding by frustrated Lewis pairs. *Angewandte Chemie - International Edition*, **2009**, 48, 6643-6	16.4	586
324	A combination of KohnSham density functional theory and multi-reference configuration interaction methods. *Journal of Chemical Physics*, **1999**, 111, 5645-5655	3.9	564
323	Rapid intramolecular heterolytic dihydrogen activation by a four-membered heterocyclic phosphane-borane adduct. *Chemical Communications*, **2007**, 5072-4	5.8	516
322	Towards chemical accuracy for the thermodynamics of large molecules: new hybrid density functionals including non-local correlation effects. *Physical Chemistry Chemical Physics*, **2006**, 8, 4398-401	3.6	476
321	Consistent structures and interactions by density functional theory with small atomic orbital basis sets. *Journal of Chemical Physics*, **2015**, 143, 054107	3.9	404
320	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	3.9	368
319	The mechanism of dihydrogen activation by frustrated Lewis pairs revisited. *Angewandte Chemie - International Edition*, **2010**, 49, 1402-5	16.4	350
318	A General Database for Main Group Thermochemistry, Kinetics, and Noncovalent Interactions - Assessment of Common and Reparameterized (meta-)GGA Density Functionals. *Journal of Chemical Theory and Computation*, **2010**, 6, 107-26	6.4	340
317	Double-hybrid density functional theory for excited electronic states of molecules. *Journal of Chemical Physics*, **2007**, 127, 154116	3.9	339
316	Report on the sixth blind test of organic crystal structure prediction methods. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2016**, 72, 439-59	1.8	338
315	Seemingly simple stereoelectronic effects in alkane isomers and the implications for Kohn-Sham density functional theory. *Angewandte Chemie - International Edition*, **2006**, 45, 4460-4	16.4	332
314	Automated exploration of the low-energy chemical space with fast quantum chemical methods. *Physical Chemistry Chemical Physics*, **2020**, 22, 7169-7192	3.6	327
313	Benchmarking of London Dispersion-Accounting Density Functional Theory Methods on Very Large Molecular Complexes. *Journal of Chemical Theory and Computation*, **2013**, 9, 1580-91	6.4	315
312	Theoretical thermodynamics for large molecules: walking the thin line between accuracy and computational cost. *Accounts of Chemical Research*, **2008**, 41, 569-79	24.3	313
311	A generally applicable atomic-charge dependent London dispersion correction. *Journal of Chemical Physics*, **2019**, 150, 154122	3.9	300
310	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, 10824-34	4.2	298
309	Extension of the D3 dispersion coefficient model. *Journal of Chemical Physics*, **2017**, 147, 034112	3.9	293
308	DFT-D3 Study of Some Molecular Crystals. *Journal of Physical Chemistry C*, **2014**, 118, 7615-7621	3.8	282

307	Corrected small basis set Hartree-Fock method for large systems. *Journal of Computational Chemistry*, **2013**, 34, 1672-85	3.5	276
306	Benchmarking density functional methods against the S66 and S66x8 datasets for non-covalent interactions. *ChemPhysChem*, **2011**, 12, 3421-33	3.2	252
305	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
304	Double-hybrid density functionals. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 576-600	7.9	227
303	B97-3c: A revised low-cost variant of the B97-D density functional method. *Journal of Chemical Physics*, **2018**, 148, 064104	3.9	221
302	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, 3067-77	2.8	211
301	How to compute isomerization energies of organic molecules with quantum chemical methods. *Journal of Organic Chemistry*, **2007**, 72, 2118-26	4.2	210
300	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, 12280-9	16.4	205
299	Metal-free catalytic olefin hydrogenation: low-temperature H2 activation by frustrated Lewis pairs. *Angewandte Chemie - International Edition*, **2012**, 51, 10164-8	16.4	200
298	Steric crowding can stabilize a labile molecule: solving the hexaphenylethane riddle. *Angewandte Chemie - International Edition*, **2011**, 50, 12639-42	16.4	197
297	Full Selectivity Control in Cobalt(III)-Catalyzed C-H Alkylations by Switching of the C-H Activation Mechanism. *Angewandte Chemie - International Edition*, **2017**, 56, 10378-10382	16.4	194
296	"Mindless" DFT Benchmarking. *Journal of Chemical Theory and Computation*, **2009**, 5, 993-1003	6.4	191
295	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, 16031-42	3.6	188
294	System-dependent dispersion coefficients for the DFT-D3 treatment of adsorption processes on ionic surfaces. *ChemPhysChem*, **2011**, 12, 3414-20	3.2	188
293	Performance of dispersion-corrected density functional theory for the interactions in ionic liquids. *Physical Chemistry Chemical Physics*, **2012**, 14, 4875-83	3.6	181
292	A simplified Tamm-Dancoff density functional approach for the electronic excitation spectra of very large molecules. *Journal of Chemical Physics*, **2013**, 138, 244104	3.9	176
291	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, 3866-71	6.4	175
290	An improved method for density functional calculations of the frequency-dependent optical rotation. *Chemical Physics Letters*, **2002**, 361, 321-328	2.5	175

289	Spin-component-scaled electron correlation methods. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 886-906	7.9	173
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287	Capture of NO by a Frustrated Lewis Pair: a new type of persistent N-oxyl radical. *Angewandte Chemie - International Edition*, **2011**, 50, 7567-71	16.4	161
286	Combinations of ethers and B(C6F5)3 function as hydrogenation catalysts. *Angewandte Chemie - International Edition*, **2013**, 52, 7492-5	16.4	160
285	Reaction of frustrated Lewis pairs with conjugated ynones-selective hydrogenation of the carbon-carbon triple bond. *Angewandte Chemie - International Edition*, **2011**, 50, 7183-6	16.4	160
284	Is spin-component scaled second-order M□ller-Plesset perturbation theory an appropriate method for the study of noncovalent interactions in molecules?. *Journal of Physical Chemistry A*, **2007**, 111, 4862-8	2.8	159
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281	Extended tight-binding quantum chemistry methods. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1493	7.9	149
280	N,N-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, 10156-68	16.4	147
279	Comprehensive Benchmark of Association (Free) Energies of Realistic Host-Guest Complexes. *Journal of Chemical Theory and Computation*, **2015**, 11, 3785-801	6.4	146
278	On the importance of the dispersion energy for the thermodynamic stability of molecules. *ChemPhysChem*, **2011**, 12, 1258-61	3.2	146
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276	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	138
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274	Reactions of phosphorus/boron frustrated Lewis pairs with SO2. *Chemical Science*, **2013**, 4, 213-219	9.4	132
273	Facile carbon monoxide reduction at intramolecular frustrated phosphane/borane Lewis pair templates. *Angewandte Chemie - International Edition*, **2013**, 52, 2243-6	16.4	132
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269	Comprehensive Thermochemical Benchmark Set of Realistic Closed-Shell Metal Organic Reactions. *Journal of Chemical Theory and Computation*, **2018**, 14, 2596-2608	6.4	122
268	Mechanism of titanocene-mediated epoxide opening through homolytic substitution. *Journal of the American Chemical Society*, **2007**, 129, 1359-71	16.4	121
267	Benchmark study of the performance of density functional theory for bond activations with (ni,pd)-based transition-metal catalysts. *ChemistryOpen*, **2013**, 2, 115-24	2.3	118
266	Formation of cyclic allenes and cumulenes by cooperative addition of frustrated Lewis pairs to conjugated enynes and diynes. *Angewandte Chemie - International Edition*, **2010**, 49, 2414-7	16.4	118
265	Towards first principles calculation of electron impact mass spectra of molecules. *Angewandte Chemie - International Edition*, **2013**, 52, 6306-12	16.4	115
264	Cation-cation "attraction": when London dispersion attraction wins over Coulomb repulsion. *Inorganic Chemistry*, **2011**, 50, 2619-28	5.1	112
263	Improved third-order Møller-Plesset perturbation theory. *Journal of Computational Chemistry*, **2003**, 24, 1529-37	3.5	111
262	Effects of London dispersion on the isomerization reactions of large organic molecules: a density functional benchmark study. *Physical Chemistry Chemical Physics*, **2010**, 12, 6940-8	3.6	110
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257	Geometrical correction for the inter- and intramolecular basis set superposition error in periodic density functional theory calculations. *Journal of Physical Chemistry A*, **2013**, 117, 9282-92	2.8	100
256	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, 8500-4	3.6	100
255	Robust Atomistic Modeling of Materials, Organometallic, and Biochemical Systems. *Angewandte Chemie - International Edition*, **2020**, 59, 15665-15673	16.4	93
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252	Calculation of the Electronic Spectra of Large Molecules. *Reviews in Computational Chemistry*, **2004**, 153-218		87
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250	Enantiomerically pure [M(6)L(12)] or [M(12)L(24)] polyhedra from flexible bis(pyridine) ligands. *Angewandte Chemie - International Edition*, **2014**, 53, 1693-8	16.4	86
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243	Carbonylation reactions of intramolecular vicinal frustrated phosphane/borane Lewis pairs. *Journal of the American Chemical Society*, **2013**, 135, 18567-74	16.4	83
242	Full Selectivity Control in Cobalt(III)-Catalyzed C▪▪I Alkylations by Switching of the C▪▪I Activation Mechanism. *Angewandte Chemie*, **2017**, 129, 10514-10518	3.6	81
241	Elucidation of the mechanism of titanocene-mediated epoxide opening by a combined experimental and theoretical approach. *Angewandte Chemie - International Edition*, **2006**, 45, 2041-4	16.4	80
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221	Blind prediction of binding affinities for charged supramolecular host-guest systems: achievements and shortcomings of DFT-D3. *Journal of Physical Chemistry B*, **2014**, 118, 3431-40	3.4	64
220	Hydrosilylation of ketones, imines and nitriles catalysed by electrophilic phosphonium cations: functional group selectivity and mechanistic considerations. *Chemistry - A European Journal*, **2015**, 21, 6491-500	4.8	63
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211	Enantiomerically pure trinuclear helicates via diastereoselective self-assembly and characterization of their redox chemistry. *Journal of the American Chemical Society*, **2014**, 136, 11830-8	16.4	55
210	Mechanistic study of the titanocene(III)-catalyzed radical arylation of epoxides. *Chemistry - A European Journal*, **2015**, 21, 280-9	4.8	54
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196	Comment on: "On the accuracy of DFT methods in reproducing ligand substitution energies for transition metal complexes in solution: the role of dispersive interactions" by H. Jacobsen and L. Cavallo. *ChemPhysChem*, **2012**, 13, 1407-9; author reply 1405-6	3.2	40
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194	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
193	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
192	Structure Optimisation of Large Transition-Metal Complexes with Extended Tight-Binding Methods. *Angewandte Chemie - International Edition*, **2019**, 58, 11078-11087	16.4	38
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