Lars Goerigk

List of Publications by Year in Descending Order

69 papers	17,146 citations	30 h-index	84 g-index
84 ext. papers	20,668 ext. citations	5.4 avg, IF	7.45 L-index

#	Paper	IF	Citations
69	Noncovalently bound excited-state dimers: a perspective on current time-dependent density functional theory approaches applied to aromatic excimer models.. *RSC Advances*, **2022**, 12, 13014-13034	3.7	4
68	CHAL336 Benchmark Set: How Well Do Quantum-Chemical Methods Describe Chalcogen-Bonding Interactions?. *Journal of Chemical Theory and Computation*, **2021**, 17, 2783-2806	6.4	18
67	A guide to benchmarking enzymatically catalysed reactions: the importance of accurate reference energies and the chemical environment. *Theoretical Chemistry Accounts*, **2021**, 140, 1	1.9	1
66	Analysis of Recent BLYP- and PBE-Based Range-Separated Double-Hybrid Density Functional Approximations for Main-Group Thermochemistry, Kinetics, and Noncovalent Interactions. *Journal of Physical Chemistry A*, **2021**, 125, 4026-4035	2.8	8
65	The Trip to the Density Functional Theory Zoo Continues: Making a Case for Time-Dependent Double Hybrids for Excited-State Problems. *Australian Journal of Chemistry*, **2021**, 74, 3	1.2	23
64	Global double hybrids do not work for charge transfer: A comment on "Double hybrids and time-dependent density functional theory: An implementation and benchmark on charge transfer excited states". *Journal of Computational Chemistry*, **2021**, 42, 528-533	3.5	9
63	The role of conformational heterogeneity in the excited state dynamics of linked diketopyrrolopyrrole dimers. *Physical Chemistry Chemical Physics*, **2021**, 23, 9357-9364	3.6	4
62	Time-Dependent Long-Range-Corrected Double-Hybrid Density Functionals with Spin-Component and Spin-Opposite Scaling: A Comprehensive Analysis of Singlet-Singlet and Singlet-Triplet Excitation Energies. *Journal of Chemical Theory and Computation*, **2021**, 17, 5165-5186	6.4	17
61	Multifunctional Coordination Polymer Exhibiting Reversible Mechanical Motion Allowing Selective Uptake of Guests and Leading to Enhanced Electrical Conductivity. *Inorganic Chemistry*, **2021**, 60, 13658-13668	5.1	0
60	A Convenient DFT-Based Strategy for Predicting Transition Temperatures of Valence Tautomeric Molecular Switches. *Inorganic Chemistry*, **2021**, 60, 14475-14487	5.1	3
59	The one-electron self-interaction error in 74 density functional approximations: a case study on hydrogenic mono- and dinuclear systems. *Physical Chemistry Chemical Physics*, **2020**, 22, 15805-15830	3.6	16
58	Semi-conducting mixed-valent X4TCNQI2II(X = H, F) charge-transfer complexes with C6H2(NH2)4. *Journal of Materials Chemistry C*, **2020**, 8, 9422-9426	7.1	2
57	Clam-like Cyclotricatechylene-based Capsules: Identifying the Roles of Protonation State and Guests as well as the Drivers for Stability and (Anti-)Cooperativity. *Chemistry - an Asian Journal*, **2020**, 15, 1301-1314	4.5	3
56	A Semiconducting Cationic Square-Grid Network with FeII Centers Displaying Unusual Dynamic Behavior. *European Journal of Inorganic Chemistry*, **2020**, 2020, 1255-1259	2.3	1
55	Structures and Magnetism of Cationic ChromiumManganese Bimetallic Oxide Clusters. *Journal of Physical Chemistry C*, **2020**, 124, 2598-2608	3.8	2
54	DFT-D4 counterparts of leading meta-generalized-gradient approximation and hybrid density functionals for energetics and geometries. *Journal of Computational Chemistry*, **2020**, 41, 2562-2572	3.5	17
53	Assessing the Tamm-Dancoff approximation, singlet-singlet, and singlet-triplet excitations with the latest long-range corrected double-hybrid density functionals.. *Journal of Chemical Physics*, **2020**, 153, 064106	3.9	29

52	Toward a Quantum-Chemical Benchmark Set for Enzymatically Catalyzed Reactions: Important Steps and Insights. *Journal of Physical Chemistry A*, **2019**, 123, 7057-7074	2.8	12
51	B2PLYP and B2GPPLYP: The First Two Double-Hybrid Density Functionals with Long-Range Correction Optimized for Excitation Energies. *Journal of Chemical Theory and Computation*, **2019**, 15, 4735-4744	6.4	55
50	Liquid Crystallinity as a Self-Assembly Motif for High-Efficiency, Solution-Processed, Solid-State Singlet Fission Materials. *Advanced Energy Materials*, **2019**, 9, 1901069	21.8	6
49	A Trip to the Density Functional Theory Zoo: Warnings and Recommendations for the User. *Australian Journal of Chemistry*, **2019**, 72, 563	1.2	77
48	Photophysical insights and guidelines for blue Turn-on Fluorescent probes for the direct detection of nitric oxide (NO) in biological systems. *Journal of Physical Organic Chemistry*, **2019**, 32, e3896	2.1	1
47	Semi-empirical or non-empirical double-hybrid density functionals: which are more robust?. *Physical Chemistry Chemical Physics*, **2018**, 20, 23175-23194	3.6	68
46	Visible-Light-Driven "On"/"Off" Photochromism of a Polyoxometalate Diarylethene Coordination Complex. *Journal of the American Chemical Society*, **2018**, 140, 10482-10487	16.4	45
45	The Nonlocal Kernel in van der Waals Density Functionals as an Additive Correction: An Extensive Analysis with Special Emphasis on the B97M-V and B97M-V Approaches. *Journal of Chemical Theory and Computation*, **2018**, 14, 5725-5738	6.4	95
44	Solution-Processable, Solid State Donor Acceptor Materials for Singlet Fission. *Advanced Energy Materials*, **2018**, 8, 1801720	21.8	15
43	A Comprehensive Assessment of the Effectiveness of Orbital Optimization in Double-Hybrid Density Functionals in the Treatment of Thermochemistry, Kinetics, and Noncovalent Interactions. *Journal of Physical Chemistry A*, **2018**, 122, 5610-5624	2.8	16
42	Non-Aqueous Microwave-Assisted Syntheses of Deca- and Hexa-Molybdovanadates. *Angewandte Chemie - International Edition*, **2017**, 56, 8568-8572	16.4	22
41	Nichtwässrige mikrowellengestützte Synthesen von Deca- und Hexamolybdovanadaten. *Angewandte Chemie*, **2017**, 129, 8691-8695	3.6	5
40	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
39	Highly Fluorescent Pyridinium Betaines for Light Harvesting. *Angewandte Chemie - International Edition*, **2017**, 56, 13882-13886	16.4	15
38	Hoch fluoreszierende Pyridiniumbetaine für die Lichtsammlung. *Angewandte Chemie*, **2017**, 129, 14070-14074	3.6	2
37	Time-Dependent Double-Hybrid Density Functionals with Spin-Component and Spin-Opposite Scaling. *Journal of Chemical Theory and Computation*, **2017**, 13, 4307-4323	6.4	41
36	Structure-reactivity correlations of the abnormal Beckmann reaction of dihydrolevoglucosenone oxime. *Organic and Biomolecular Chemistry*, **2017**, 15, 10105-10115	3.9	4
35	A Comprehensive Overview of the DFT-D3 London-Dispersion Correction **2017**, 195-219		27

34	On the inclusion of post-MP2 contributions to double-hybrid density functionals. *Journal of Computational Chemistry*, **2016**, 37, 183-93	3.5	25
33	Problems, successes and challenges for the application of dispersion-corrected density-functional theory combined with dispersion-based implicit solvent models to large-scale hydrophobic self-assembly and polymorphism. *Molecular Simulation*, **2016**, 42, 494-510	2	13
32	From Chaos to Order: Chain-Length Dependence of the Free Energy of Formation of Meso-tetraalkylporphyrin Self-Assembled Monolayer Polymorphs. *Journal of Physical Chemistry C*, **2016**, 120, 1739-1748	3.8	13
31	The INV24 test set: how well do quantum-chemical methods describe inversion and racemization barriers?. *Canadian Journal of Chemistry*, **2016**, 94, 1133-1143	0.9	28
30	Photoisomerization action spectroscopy: flicking the protonated merocyanine-spiropyran switch in the gas phase. *Physical Chemistry Chemical Physics*, **2015**, 17, 25676-88	3.6	38
29	A priori calculations of the free energy of formation from solution of polymorphic self-assembled monolayers. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, E6101-10	11.5	32
28	Treating London-Dispersion Effects with the Latest Minnesota Density Functionals: Problems and Possible Solutions. *Journal of Physical Chemistry Letters*, **2015**, 6, 3891-6	6.4	67
27	A Heteroaromatically Functionalized Hexamolybdate. *Inorganics*, **2015**, 3, 82-100	2.9	5
26	Accurate reaction barrier heights of pericyclic reactions: Surprisingly large deviations for the CBS-QB3 composite method and their consequences in DFT benchmark studies. *Journal of Computational Chemistry*, **2015**, 36, 622-32	3.5	92
25	How Do DFT-DCP, DFT-NL, and DFT-D3 Compare for the Description of London-Dispersion Effects in Conformers and General Thermochemistry?. *Journal of Chemical Theory and Computation*, **2014**, 10, 968-80	6.4	69
24	Double-hybrid density functionals. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 576-600	7.9	227
23	Recommending Hartree-Fock theory with London-dispersion and basis-set-superposition corrections for the optimization or quantum refinement of protein structures. *Journal of Physical Chemistry B*, **2014**, 118, 14612-26	3.4	46
22	Accurate quantum chemical energies for tetrapeptide conformations: why MP2 data with an insufficient basis set should be handled with caution. *Physical Chemistry Chemical Physics*, **2013**, 15, 7028-31	3.6	57
21	Efficient Methods for the Quantum Chemical Treatment of Protein Structures: The Effects of London-Dispersion and Basis-Set Incompleteness on Peptide and Water-Cluster Geometries. *Journal of Chemical Theory and Computation*, **2013**, 9, 3240-51	6.4	61
20	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
19	Theoretical Electronic Circular Dichroism Spectroscopy of Large Organic and Supramolecular Systems **2012**, 643-673		16
18	Spin-component-scaled electron correlation methods. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 886-906	7.9	173
17	Why the Standard B3LYP/6-31G* Model Chemistry Should Not Be Used in DFT Calculations of Molecular Thermochemistry: Understanding and Correcting the Problem. *Journal of Organic Chemistry*, **2012**, 77, 10824-10834	4.2	1

16	First Steps Towards Quantum Refinement of Protein X-Ray Structures **2012**, 87-120		6
15	Accurate Dispersion-Corrected Density Functionals for General Chemistry Applications **2011**, 1-16		1
14	Double-Hybrid Density Functionals Provide a Balanced Description of Excited (1)La and (1)Lb States in Polycyclic Aromatic Hydrocarbons. *Journal of Chemical Theory and Computation*, **2011**, 7, 3272-7	6.4	72
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. *Journal of Chemical Theory and Computation*, **2011**, 7, 291-309	6.4	841
12	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
11	Benchmarking density functional methods against the S66 and S66x8 datasets for non-covalent interactions. *ChemPhysChem*, **2011**, 12, 3421-33	3.2	252
10	Effect of the damping function in dispersion corrected density functional theory. *Journal of Computational Chemistry*, **2011**, 32, 1456-65	3.5	10429
9	Assessment of TD-DFT methods and of various spin scaled CIS(D) and CC2 versions for the treatment of low-lying valence excitations of large organic dyes. *Journal of Chemical Physics*, **2010**, 132, 184103	3.9	282
8	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
7	Neue Einblicke in den Mechanismus der Diwasserstoff-Aktivierung durch frustrierte Lewis-Paare. *Angewandte Chemie*, **2010**, 122, 1444-1447	3.6	110
6	The mechanism of dihydrogen activation by frustrated Lewis pairs revisited. *Angewandte Chemie - International Edition*, **2010**, 49, 1402-5	16.4	350
5	Computation of accurate excitation energies for large organic molecules with double-hybrid density functionals. *Physical Chemistry Chemical Physics*, **2009**, 11, 4611-20	3.6	224
4	Calculation of electronic circular dichroism spectra with time-dependent double-hybrid density functional theory. *Journal of Physical Chemistry A*, **2009**, 113, 767-76	2.8	120
3	Optimization and basis-set dependence of a restricted-open-shell form of B2-PLYP double-hybrid density functional theory. *Journal of Physical Chemistry A*, **2009**, 113, 9861-73	2.8	70
2	Quantum chemical investigation of exciton coupling: super-molecular calculations of a merocyanine dimer aggregate. *ChemPhysChem*, **2008**, 9, 2467-70	3.2	30
1	The CHAL336 Benchmark Set: How Well Do Quantum-Chemical Methods Describe Chalcogen-Bonding Interactions?		3