Lars Goerigk

List of Publications by Year
in descending order

68 papers	24,794 citations	101543 36 h-index	98798 67 g-index
84 all docs	84 docs citations	84 times ranked	24330 citing authors

#	Article	IF	Citations
1	Effect of the damping function in dispersion corrected density functional theory. Journal of Computational Chemistry, 2011, 32, 1456-1465.	3.3	15,980
2	A thorough benchmark of density functional methods for general main group thermochemistry, kinetics, and noncovalent interactions. Physical Chemistry Chemical Physics, 2011, 13, 6670.	2.8	1,627
3	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.	2.8	1,230
4	Efficient and Accurate Double-Hybrid-Meta-GGA Density Functionalsâ€”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.	5.3	1,035
5	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.	3.2	407
6	The Mechanism of Dihydrogen Activation by Frustrated Lewis Pairs Revisited. Angewandte Chemie - International Edition, 2010, 49, 1402-1405.	13.8	394
7	A General Database for Main Group Thermochemistry, Kinetics, and Noncovalent Interactions âˆ’ Assessment of Common and Reparameterized (<i>meta</i>-)GGA Density Functionals. Journal of Chemical Theory and Computation, 2010, 6, 107-126.	5.3	389
8	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, .	3.0	313
9	Doubleâ€hybrid density functionals. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 576-600.	14.6	292
10	Benchmarking Density Functional Methods against the S66 and S66x8 Datasets for Nonâ€Covalent Interactions. ChemPhysChem, 2011, 12, 3421-3433.	2.1	283
11	Computation of accurate excitation energies for large organic molecules with double-hybrid density functionals. Physical Chemistry Chemical Physics, 2009, 11, 4611.	2.8	252
12	Spinâ€componentâ€scaled electron correlation methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 886-906.	14.6	197
13	The Nonlocal Kernel in van der Waals Density Functionals as an Additive Correction: An Extensive Analysis with Special Emphasis on the B97M-V and Ï‰B97M-V Approaches. Journal of Chemical Theory and Computation, 2018, 14, 5725-5738.	5.3	170
14	Calculation of Electronic Circular Dichroism Spectra with Time-Dependent Double-Hybrid Density Functional Theory. Journal of Physical Chemistry A, 2009, 113, 767-776.	2.5	133
15	Accurate reaction barrier heights of pericyclic reactions: Surprisingly large deviations for the <scp>CBSâ€QB3</scp> composite method and their consequences in <scp>DFT</scp> benchmark studies. Journal of Computational Chemistry, 2015, 36, 622-632.	3.3	124
16	A Trip to the Density Functional Theory Zoo: Warnings and Recommendations for the User. Australian Journal of Chemistry, 2019, 72, 563.	0.9	115
17	Ï‰B2PLYP and Ï‰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.	5.3	107
18	Semi-empirical or non-empirical double-hybrid density functionals: which are more robust?. Physical Chemistry Chemical Physics, 2018, 20, 23175-23194.	2.8	102

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19	Treating London-Dispersion Effects with the Latest Minnesota Density Functionals: Problems and Possible Solutions. Journal of Physical Chemistry Letters, 2015, 6, 3891-3896.	4.6	91
20	Double-Hybrid Density Functionals Provide a Balanced Description of Excited ¹L_a and ¹L_b States in Polycyclic Aromatic Hydrocarbons. Journal of Chemical Theory and Computation, 2011, 7, 3272-3277.	5.3	84
21	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, 968-980.	5.3	81
22	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, 9861-9873.	2.5	77
23	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, 3240-3251.	5.3	75
24	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.	2.8	67
25	DFT<scp>â€Ð4</scp> counterparts of leading <scp>metaâ€</scp>generalizedâ€gradient approximation and hybrid density functionals for energetics and geometries. Journal of Computational Chemistry, 2020, 41, 2562-2572.	3.3	61
26	Time-Dependent Double-Hybrid Density Functionals with Spin-Component and Spin-Opposite Scaling. Journal of Chemical Theory and Computation, 2017, 13, 4307-4323.	5.3	60
27	Visible-Light-Driven â€œOnâ€/â€œOffâ€•Photochromism of a Polyoxometalate Diarylethene Coordination Complex. Journal of the American Chemical Society, 2018, 140, 10482-10487.	13.7	60
28	Time-Dependent Long-Range-Corrected Double-Hybrid Density Functionals with Spin-Component and Spin-Opposite Scaling: A Comprehensive Analysis of Singletâ€“Singlet and Singletâ€“Triplet Excitation Energies. Journal of Chemical Theory and Computation, 2021, 17, 5165-5186.	5.3	58
29	A Comprehensive Overview of the DFT-D3 London-Dispersion Correction. , 2017, , 195-219.		57
30	Assessing the Tammâ€“Dancoff approximation, singletâ€“singlet, and singletâ€“triplet excitations with the latest long-range corrected double-hybrid density functionals. Journal of Chemical Physics, 2020, 153, 064106.	3.0	54
31	Recommending Hartreeâ€“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, 14612-14626.	2.6	53
32	Photoisomerization action spectroscopy: flicking the protonated merocyanineâ€“spiropyran switch in the gas phase. Physical Chemistry Chemical Physics, 2015, 17, 25676-25688.	2.8	46
33	The INV24 test set: how well do quantum-chemical methods describe inversion and racemization barriers?. Canadian Journal of Chemistry, 2016, 94, 1133-1143.	1.1	45
34	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.	7.1	42
35	CHAL336 Benchmark Set: How Well Do Quantum-Chemical Methods Describe Chalcogen-Bonding Interactions?. Journal of Chemical Theory and Computation, 2021, 17, 2783-2806.	5.3	42
36	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.	0.9	39

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37	Quantum Chemical Investigation of Exciton Coupling: Superâ€Molecular Calculations of a Merocyanine Dimer Aggregate. ChemPhysChem, 2008, 9, 2467-2470.	2.1	34
38	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.	2.5	31
39	On the inclusion of postâ€<scp>MP</scp>2 contributions to doubleâ€Hybrid density functionals. Journal of Computational Chemistry, 2016, 37, 183-193.	3.3	30
40	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.	2.8	27
41	Nonâ€Aqueous Microwaveâ€Assisted Syntheses of Decaâ€•and Hexaâ€Molybdovanadates. Angewandte Chemie - International Edition, 2017, 56, 8568-8572.	13.8	25
42	Solutionâ€Processable, Solid State Donorâ€“Acceptor Materials for Singlet Fission. Advanced Energy Materials, 2018, 8, 1801720.	19.5	21
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.	2.5	19
44	Toward a Quantum-Chemical Benchmark Set for Enzymatically Catalyzed Reactions: Important Steps and Insights. Journal of Physical Chemistry A, 2019, 123, 7057-7074.	2.5	19
45	Highly Fluorescent Pyridinium Betaines for Light Harvesting. Angewandte Chemie - International Edition, 2017, 56, 13882-13886.	13.8	18
46	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.	3.6	18
47	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.	3.1	16
48	Global double hybrids do not work for charge transfer: A comment on â€œDouble hybrids and timeâ€dependent density functional theory: An implementation and benchmark on charge transfer excited statesâ€. Journal of Computational Chemistry, 2021, 42, 528-533.	3.3	15
49	A Convenient DFT-Based Strategy for Predicting Transition Temperatures of Valence Tautomeric Molecular Switches. Inorganic Chemistry, 2021, 60, 14475-14487.	4.0	14
50	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.	3.2	14
51	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.	2.0	13
52	The role of conformational heterogeneity in the excited state dynamics of linked diketopyrrolopyrrole dimers. Physical Chemistry Chemical Physics, 2021, 23, 9357-9364.	2.8	12
53	Structureâ€“reactivity correlations of the abnormal Beckmann reaction of dihydrolevoglucosenone oxime. Organic and Biomolecular Chemistry, 2017, 15, 10105-10115.	2.8	11
54	Liquid Crystallinity as a Selfâ€Assembly Motif for Highâ€Efficiency, Solutionâ€Processed, Solidâ€State Singlet Fission Materials. Advanced Energy Materials, 2019, 9, 1901069.	19.5	11

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55	A Heteroaromatically Functionalized Hexamolybdate. Inorganics, 2015, 3, 82-100.	2.7	7
56	First Steps Towards Quantum Refinement of Protein X-Ray Structures. , 2012, , 87-120.		7
57	A guide to benchmarking enzymatically catalysed reactions: the importance of accurate reference energies and the chemical environment. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	6
58	NichtwÃ¤ssrige mikrowellengestÃ¼tzte Synthesen von Decaâ€•und Hexamolybdovanadaten. Angewandte Chemie, 2017, 129, 8691-8695.	2.0	5
59	Photophysical insights and guidelines for blue â€œturnâ€onâ€•fluorescent probes for the direct detection of nitric oxide (NO^{â€¢}) in biological systems. Journal of Physical Organic Chemistry, 2019, 32, e3896.	1.9	5
60	Multifunctional Coordination Polymer Exhibiting Reversible Mechanical Motion Allowing Selective Uptake of Guests and Leading to Enhanced Electrical Conductivity. Inorganic Chemistry, 2021, 60, 13658-13668.	4.0	5
61	Semi-conducting mixed-valent X₄TCNQ^{Iâˆ’/IIâˆ’} (X = H, F) charge-transfer complexes with C₆H₂(NH₂)₄. Journal of Materials Chemistry C, 2020, 8, 9422-9426.	5.5	4
62	Clamâ€like Cyclotricatechyleneâ€based Capsules: Identifying the Roles of Protonation State and Guests as well as the Drivers for Stability and (Antiâ€)Cooperativity. Chemistry - an Asian Journal, 2020, 15, 1301-1314.	3.3	4
63	Assessing Recent Time-Dependent Double-Hybrid Density Functionals on Doubletâ€"Doublet Excitations. ACS Physical Chemistry Au, 2022, 2, 407-416.	4.0	3
64	Accurate Dispersion-Corrected Density Functionals for General Chemistry Applications. , 2011, , 1-16.		2
65	Hoch fluoreszierende Pyridiniumbetaine fÃ¼r die Lichtsammlung. Angewandte Chemie, 2017, 129, 14070-14074.	2.0	2
66	Structures and Magnetism of Cationic Chromiumâ€"Manganese Bimetallic Oxide Clusters. Journal of Physical Chemistry C, 2020, 124, 2598-2608.	3.1	2
67	Assessing the Applicability of the Geometric Counterpoise Correction in B2PLYP/Double-Î¶ Calculations for Thermochemistry, Kinetics, and Noncovalent Interactions*. Australian Journal of Chemistry, 2021, , .	0.9	2
68	A Semiconducting Cationic Squareâ€Grid Network with Fe III Centers Displaying Unusual Dynamic Behavior. European Journal of Inorganic Chemistry, 2020, 2020, 1255-1259.	2.0	1