# Lars Goerigk

List of Publications by Year
in descending order

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

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | 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 |
| 2 | Assessing Recent Time-Dependent Double-Hybrid Density Functionals on Doubletâ€“Doublet Excitations. ACS Physical Chemistry Au, 2022, 2, 407-416. | 4.0 | 3 |
| 3 | 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 |
| 4 | 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 |
| 5 | 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 |
| 6 | 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 |
| 7 | 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 |
| 8 | 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 |
| 9 | 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 |
| 10 | 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 |
| 11 | 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 |
| 12 | A Convenient DFT-Based Strategy for Predicting Transition Temperatures of Valence Tautomeric Molecular Switches. Inorganic Chemistry, 2021, 60, 14475-14487. | 4.0 | 14 |
| 13 | Structures and Magnetism of Cationic Chromiumâ€“Manganese Bimetallic Oxide Clusters. Journal of Physical Chemistry C, 2020, 124, 2598-2608. | 3.1 | 2 |
| 14 | DFT<scp>â€D4</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 |
| 15 | 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 |
| 16 | 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 |
| 17 | Semi-conducting mixed-valent X<sub>4</sub>TCNQ<sup>Iâ€²/IIâ€²</sup> (X = H, F) charge-transfer complexes with C<sub>6</sub>H<sub>2</sub>(NH<sub>2</sub>)<sub>4</sub>. Journal of Materials Chemistry C, 2020, 8, 9422-9426. | 5.5 | 4 |
| 18 | Clamâ€like Cyclotricatecheleneâ€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 |

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| 19 | 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 |
| 20 | 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 |
| 21 | 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 |
| 22 | 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 |
| 23 | A Trip to the Density Functional Theory Zoo: Warnings and Recommendations for the User. Australian Journal of Chemistry, 2019, 72, 563. | 0.9 | 115 |
| 24 | Photophysical insights and guidelines for blue â€œturnâ€onâ€•fluorescent probes for the direct detection of nitric oxide (NO<sup>â€¢</sup>) in biological systems. Journal of Physical Organic Chemistry, 2019, 32, e3896. | 1.9 | 5 |
| 25 | 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 |
| 26 | Solutionâ€Processable, Solid State Donorâ€“Acceptor Materials for Singlet Fission. Advanced Energy Materials, 2018, 8, 1801720. | 19.5 | 21 |
| 27 | 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 |
| 28 | Semi-empirical or non-empirical double-hybrid density functionals: which are more robust?. Physical Chemistry Chemical Physics, 2018, 20, 23175-23194. | 2.8 | 102 |
| 29 | 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 |
| 30 | Nonâ€Aqueous Microwaveâ€Assisted Syntheses of Decaâ€•and Hexaâ€Molybdovanadates. Angewandte Chemie - International Edition, 2017, 56, 8568-8572. | 13.8 | 25 |
| 31 | NichtwÃssrige mikrowellengestÃ¼tzte Synthesen von Decaâ€•und Hexamolybdovanadaten. Angewandte Chemie, 2017, 129, 8691-8695. | 2.0 | 5 |
| 32 | 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 |
| 33 | Highly Fluorescent Pyridinium Betaines for Light Harvesting. Angewandte Chemie - International Edition, 2017, 56, 13882-13886. | 13.8 | 18 |
| 34 | Hoch fluoreszierende Pyridiniumbetaine fÃ¼r die Lichtsammlung. Angewandte Chemie, 2017, 129, 14070-14074. | 2.0 | 2 |
| 35 | 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 |
| 36 | Structureâ€“reactivity correlations of the abnormal Beckmann reaction of dihydrolevoglucosenone oxime. Organic and Biomolecular Chemistry, 2017, 15, 10105-10115. | 2.8 | 11 |

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|---|---|---|---|
| 37 | A Comprehensive Overview of the DFT-D3 London-Dispersion Correction. , 2017, , 195-219. | | 57 |
| 38 | 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 |
| 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 | 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 |
| 41 | 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 |
| 42 | A Heteroaromatically Functionalized Hexamolybdate. Inorganics, 2015, 3, 82-100. | 2.7 | 7 |
| 43 | 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 |
| 44 | Photoisomerization action spectroscopy: flicking the protonated merocyanineâ€“spiropyran switch in the gas phase. Physical Chemistry Chemical Physics, 2015, 17, 25676-25688. | 2.8 | 46 |
| 45 | 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 |
| 46 | 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 |
| 47 | 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 |
| 48 | 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 |
| 49 | Doubleâ€hybrid density functionals. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 576-600. | 14.6 | 292 |
| 50 | 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 |
| 51 | 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 |
| 52 | 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 |
| 53 | Spinâ€componentâ€scaled electron correlation methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 886-906. | 14.6 | 197 |
| 54 | First Steps Towards Quantum Refinement of Protein X-Ray Structures. , 2012, , 87-120. | | 7 |

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| 55 | 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 |
| 56 | Accurate Dispersion-Corrected Density Functionals for General Chemistry Applications. , 2011, , 1-16. | | 2 |
| 57 | Double-Hybrid Density Functionals Provide a Balanced Description of Excited <sup>1</sup>L<sub>a</sub> and <sup>1</sup>L<sub>b</sub> States in Polycyclic Aromatic Hydrocarbons. Journal of Chemical Theory and Computation, 2011, 7, 3272-3277. | 5.3 | 84 |
| 58 | 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 |
| 59 | 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 |
| 60 | Benchmarking Density Functional Methods against the S66 and S66x8 Datasets for Nonâ€Covalent Interactions. ChemPhysChem, 2011, 12, 3421-3433. | 2.1 | 283 |
| 61 | Effect of the damping function in dispersion corrected density functional theory. Journal of Computational Chemistry, 2011, 32, 1456-1465. | 3.3 | 15,980 |
| 62 | The Mechanism of Dihydrogen Activation by Frustrated Lewis Pairs Revisited. Angewandte Chemie - International Edition, 2010, 49, 1402-1405. | 13.8 | 394 |
| 63 | 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 |
| 64 | A General Database for Main Group Thermochemistry, Kinetics, and Noncovalent Interactions â˜' Assessment of Common and Reparameterized (meta-)GGA Density Functionals. Journal of Chemical Theory and Computation, 2010, 6, 107-126. | 5.3 | 389 |
| 65 | Computation of accurate excitation energies for large organic molecules with double-hybrid density functionals. Physical Chemistry Chemical Physics, 2009, 11, 4611. | 2.8 | 252 |
| 66 | 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 |
| 67 | 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 |
| 68 | Quantum Chemical Investigation of Exciton Coupling: Superâ€Molecular Calculations of a Merocyanine Dimer Aggregate. ChemPhysChem, 2008, 9, 2467-2470. | 2.1 | 34 |