Robin Grotjahn

List of Publications by Year
in descending order

12	853	933447 10	1199594 12
papers	citations	h-index	g-index

12	12	12	1063
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. Journal of Chemical Physics, 2020, 152, 184107.	3.0	616
2	Development of a TDDFT-Based Protocol with Local Hybrid Functionals for the Screening of Potential Singlet Fission Chromophores. Journal of Chemical Theory and Computation, 2017, 13, 4984-4996.	5.3	57
3	A Local Hybrid Functional with Wide Applicability and Good Balance between (De)Localization and Leftâ€“Right Correlation. Journal of Chemical Theory and Computation, 2020, 16, 5645-5657.	5.3	54
4	Development and Implementation of Excited-State Gradients for Local Hybrid Functionals. Journal of Chemical Theory and Computation, 2019, 15, 5508-5522.	5.3	21
5	Validation of Local Hybrid Functionals for Excited States: Structures, Fluorescence, Phosphorescence, and Vibronic Spectra. Journal of Chemical Theory and Computation, 2020, 16, 5821-5834.	5.3	21
6	Two Ï€â€Electrons Make the Difference: From BODIPY to BODIIM Switchable Fluorescent Dyes. Chemistry - A European Journal, 2020, 26, 1422-1428.	3.3	18
7	Evaluation of Local Hybrid Functionals for Electric Properties: Dipole Moments and Static and Dynamic Polarizabilities. Journal of Physical Chemistry A, 2020, 124, 8346-8358.	2.5	15
8	Assessment of hybrid functionals for singlet and triplet excitations: Why do some local hybrid functionals perform so well for triplet excitation energies?. Journal of Chemical Physics, 2021, 155, 124108.	3.0	14
9	Reliable TDDFT Protocol Based on a Local Hybrid Functional for the Prediction of Vibronic Phosphorescence Spectra Applied to Tris(2,2â€²-bipyridine)-Metal Complexes. Journal of Physical Chemistry A, 2021, 125, 7099-7110.	2.5	13
10	Electronic States of 2,3-Diamino-1,4-naphthoquinone and Its N-Alkylated Derivatives. Journal of Physical Chemistry C, 2020, 124, 60-69.	3.1	12
11	A Look at Realâ€World Transitionâ€Metal Thermochemistry and Kinetics with Local Hybrid Functionals. Israel Journal of Chemistry, 2023, 63, .	2.3	8
12	A novel model for smectic liquid crystals: Elastic anisotropy and response to a steady-state flow. Journal of Chemical Physics, 2016, 145, 164903.	3.0	4