Toni M Maier

List of Publications by Year
in descending order

13	524	933447 10	1125743 13
papers	citations	h-index	g-index

13	13	13	406
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Assessing locally range-separated hybrid functionals from a gradient expansion of the exchange energy density. Journal of Chemical Physics, 2021, 154, 214101.	3.0	10
2	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
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	Relativistic local hybrid functionals and their impact on 1s core orbital energies. Journal of Chemical Physics, 2020, 152, 214103.	3.0	7
5	Local hybrid functionals: Theory, implementation, and performance of an emerging new tool in quantum chemistry and beyond. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1378.	14.6	95
6	Restoring the iso-orbital limit of the kinetic energy density in relativistic density functional theory. Journal of Chemical Physics, 2019, 151, 174114.	3.0	7
7	Efficient Semi-Numerical Implementation of Relativistic Exact Exchange within the Infinite-Order Two-Component Method Using a Modified Chain-of-Spheres Method. Journal of Chemical Theory and Computation, 2019, 15, 4745-4763.	5.3	13
8	Lessons from the Spin-Polarization/Spin-Contamination Dilemma of Transition-Metal Hyperfine Couplings for the Construction of Exchange-Correlation Functionals. Journal of Chemical Theory and Computation, 2018, 14, 5653-5672.	5.3	35
9	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
10	Validation of local hybrid functionals for TDDFT calculations of electronic excitation energies. Journal of Chemical Physics, 2016, 144, 074106.	3.0	117
11	New approaches for the calibration of exchange-energy densities in local hybrid functionals. Physical Chemistry Chemical Physics, 2016, 18, 21133-21144.	2.8	43
12	Efficient Semi-numerical Implementation of Global and Local Hybrid Functionals for Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2015, 11, 4226-4237.	5.3	54
13	The vibrational spectrum of FeO2+ isomersâ€”Theoretical benchmark and experiment. Journal of Chemical Physics, 2014, 140, 204315.	3.0	20