

Toni M Maier

List of Publications by Year in descending order

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13
papers

524
citations

933447

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1125743

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13
docs citations

13
times ranked

406
citing authors

#	ARTICLE	IF	CITATIONS
1	Validation of local hybrid functionals for TDDFT calculations of electronic excitation energies. <i>Journal of Chemical Physics</i> , 2016, 144, 074106.	3.0	117
2	Local hybrid functionals: Theory, implementation, and performance of an emerging new tool in quantum chemistry and beyond. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2019, 9, e1378.	14.6	95
3	Development of a TDDFT-Based Protocol with Local Hybrid Functionals for the Screening of Potential Singlet Fission Chromophores. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4984-4996.	5.3	57
4	Efficient Semi-numerical Implementation of Global and Local Hybrid Functionals for Time-Dependent Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4226-4237.	5.3	54
5	A Local Hybrid Functional with Wide Applicability and Good Balance between (De)Localization and Left-Right Correlation. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5645-5657.	5.3	54
6	New approaches for the calibration of exchange-energy densities in local hybrid functionals. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21133-21144.	2.8	43
7	Lessons from the Spin-Polarization/Spin-Contamination Dilemma of Transition-Metal Hyperfine Couplings for the Construction of Exchange-Correlation Functionals. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5653-5672.	5.3	35
8	The vibrational spectrum of FeO ₂ ⁺ isomers – Theoretical benchmark and experiment. <i>Journal of Chemical Physics</i> , 2014, 140, 204315.	3.0	20
9	Efficient Semi-Numerical Implementation of Relativistic Exact Exchange within the Infinite-Order Two-Component Method Using a Modified Chain-of-Spheres Method. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4745-4763.	5.3	13
10	Electronic States of 2,3-Diamino-1,4-naphthoquinone and Its N-Alkylated Derivatives. <i>Journal of Physical Chemistry C</i> , 2020, 124, 60-69.	3.1	12
11	Assessing locally range-separated hybrid functionals from a gradient expansion of the exchange energy density. <i>Journal of Chemical Physics</i> , 2021, 154, 214101.	3.0	10
12	Restoring the iso-orbital limit of the kinetic energy density in relativistic density functional theory. <i>Journal of Chemical Physics</i> , 2019, 151, 174114.	3.0	7
13	Relativistic local hybrid functionals and their impact on 1s core orbital energies. <i>Journal of Chemical Physics</i> , 2020, 152, 214103.	3.0	7