

GrÃ©goire David

List of Publications by Year in descending order

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419
citing authors

#	ARTICLE	IF	CITATIONS
1	Optimizing Molecular Geometries in Strong Magnetic Fields. Journal of Chemical Theory and Computation, 2021, 17, 2166-2185.	5.3	29
2	Self-Consistent Field Methods for Excited States in Strong Magnetic Fields: a Comparison between Energy- and Variance-Based Approaches. Journal of Chemical Theory and Computation, 2021, 17, 5492-5508.	5.3	16
3	Analyzing Magnetically Induced Currents in Molecular Systems Using Current-Density-Functional Theory. Journal of Physical Chemistry A, 2020, 124, 1321-1333.	2.5	42
4	Consistent spin decontamination of broken-symmetry calculations of diradicals. Journal of Chemical Physics, 2020, 153, 194107.	3.0	11
5	Improved evaluation of spin-polarization energy contributions using broken-symmetry calculations. Journal of Chemical Physics, 2020, 153, 054120.	3.0	9
6	Quantum Package 2.0: An Open-Source Determinant-Driven Suite of Programs. Journal of Chemical Theory and Computation, 2019, 15, 3591-3609.	5.3	108
7	Chemical Tuning of Magnetic Exchange Couplings Using Broken-Symmetry Density Functional Theory. Inorganic Chemistry, 2018, 57, 12769-12776.	4.0	32
8	Qualitative Views on the Polyradical Character of Long Acenes. Journal of Physical Chemistry A, 2018, 122, 6926-6933.	2.5	28
9	What Are the Physical Contents of Hubbard and Heisenberg Hamiltonian Interactions Extracted from Broken Symmetry DFT Calculations in Magnetic Compounds?. Journal of Chemical Theory and Computation, 2017, 13, 6253-6265.	5.3	16
10	Scrutinizing "Invisible" states: A challenge for modern density functionals. Journal of Computational Chemistry, 2016, 37, 1345-1354.	3.3	42
11	Difficulty of the evaluation of the barrier height of an open-shell transition state between closed shell minima: the case of small C _{4n} rings. Journal of Chemical Physics, 0, , .	3.0	2