

Abel Carreras

List of Publications by Year in descending order

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Version: 2024-02-01

20
papers

953
citations

933447

10
h-index

794594

19
g-index

22
all docs

22
docs citations

22
times ranked

1194
citing authors

#	ARTICLE	IF	CITATIONS
1	Simple evaluation of dynamic disorder effects on exciton transport. <i>Journal of Chemical Physics</i> , 2022, 156, 044112.	3.0	0
2	Theory of Exciton Dynamics in Thermally Activated Delayed Fluorescence. <i>ChemPhotoChem</i> , 2022, 6, .	3.0	1
3	Short-range DFT energy correction to multiconfigurational wave functions for open-shell systems. <i>Journal of Chemical Physics</i> , 2021, 154, 124116.	3.0	5
4	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	3.0	518
5	Calculation of spin-orbit couplings using RASCI spinless one-particle density matrices: Theory and applications. <i>Journal of Chemical Physics</i> , 2020, 153, 214107.	3.0	18
6	Effects of Temperature on the Shape and Symmetry of Molecules and Solids. <i>Chemistry - A European Journal</i> , 2019, 25, 673-691.	3.3	5
7	Singlet fission in spiroconjugated dimers. <i>Journal of Chemical Physics</i> , 2019, 150, 204306.	3.0	23
8	Conformational analysis of enantiomerization coupled to internal rotation in triptycyl-n-helicenes. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 11395-11404.	2.8	1
9	Charge Delocalization, Oxidation States, and Silver Mobility in the Mixed Silver-Copper Oxide AgCuO_2 . <i>Inorganic Chemistry</i> , 2019, 58, 7026-7035.	4.0	5
10	Photophysics of Molecular Aggregates from Excited State Diabatization. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2320-2330.	5.3	11
11	Triangular graphene nanofragments: open-shell character and doping. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9069-9076.	2.8	41
12	Cholesteric Aggregation at the Quinoidal-to-Diradical Border Enabled Stable n-Doped Conductor. <i>CheM</i> , 2019, 5, 964-976.	11.7	79
13	Temperature-dependent phonon spectra of magnetic random solid solutions. <i>Npj Computational Materials</i> , 2018, 4, .	8.7	19
14	Mode decomposition based on crystallographic symmetry in the band-unfolding method. <i>Physical Review B</i> , 2017, 95, .	3.2	46
15	DynaPhoPy: A code for extracting phonon quasiparticles from molecular dynamics simulations. <i>Computer Physics Communications</i> , 2017, 221, 221-234.	7.5	105
16	Atomistic Origin of Phase Stability in Oxygen-Functionalized MXene: A Comparative Study. <i>Journal of Physical Chemistry C</i> , 2017, 121, 18947-18953.	3.1	44
17	A push-pull organic dye with a quinoidal thiophene linker: Photophysical properties and solvent effects. <i>Chemical Physics Letters</i> , 2016, 663, 45-50.	2.6	3
18	A fullerene-carbene adduct as a crystalline molecular rotor: remarkable behavior of a spherically-shaped rotator. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 12980-12986.	2.8	8

#	ARTICLE	IF	CITATIONS
19	Pseudosymmetry analysis of molecular orbitals. <i>Journal of Computational Chemistry</i> , 2013, 34, 1321-1331.	3.3	7
20	Concurrent Symmetries: The Interplay Between Local and Global Molecular Symmetries. <i>Chemistry - A European Journal</i> , 2011, 17, 359-367.	3.3	14