Abel Carreras

List of Publications by Year
in descending order

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	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
2	DynaPhoPy: A code for extracting phonon quasiparticles from molecular dynamics simulations. Computer Physics Communications, 2017, 221, 221-234.	7.5	105
3	Cholesteric Aggregation at the Quinoidal-to-Diradical Border Enabled Stable n-Doped Conductor. CheM, 2019, 5, 964-976.	11.7	79
4	Mode decomposition based on crystallographic symmetry in the band-unfolding method. Physical Review B, 2017, 95, .	3.2	46
5	Atomistic Origin of Phase Stability in Oxygen-Functionalized MXene: A Comparative Study. Journal of Physical Chemistry C, 2017, 121, 18947-18953.	3.1	44
6	Triangular graphene nanofragments: open-shell character and doping. Physical Chemistry Chemical Physics, 2019, 21, 9069-9076.	2.8	41
7	Singlet fission in spiroconjugated dimers. Journal of Chemical Physics, 2019, 150, 204306.	3.0	23
8	Temperature-dependent phonon spectra of magnetic random solid solutions. Npj Computational Materials, 2018, 4, .	8.7	19
9	Calculation of spinâ€“orbit couplings using RASCI spinless one-particle density matrices: Theory and applications. Journal of Chemical Physics, 2020, 153, 214107.	3.0	18
10	Concurrent Symmetries: The Interplay Between Local and Global Molecular Symmetries. Chemistry - A European Journal, 2011, 17, 359-367.	3.3	14
11	Photophysics of Molecular Aggregates from Excited State Diabatization. Journal of Chemical Theory and Computation, 2019, 15, 2320-2330.	5.3	11
12	A fullereneâ€“carbene adduct as a crystalline molecular rotor: remarkable behavior of a spherically-shaped rotator. Physical Chemistry Chemical Physics, 2014, 16, 12980-12986.	2.8	8
13	Pseudosymmetry analysis of molecular orbitals. Journal of Computational Chemistry, 2013, 34, 1321-1331.	3.3	7
14	Effects of Temperature on the Shape and Symmetry of Molecules and Solids. Chemistry - A European Journal, 2019, 25, 673-691.	3.3	5
15	Charge Delocalization, Oxidation States, and Silver Mobility in the Mixed Silverâ€“Copper Oxide AgCuO₂. Inorganic Chemistry, 2019, 58, 7026-7035.	4.0	5
16	Short-range DFT energy correction to multiconfigurational wave functions for open-shell systems. Journal of Chemical Physics, 2021, 154, 124116.	3.0	5
17	A push-pull organic dye with a quinoidal thiophene linker: Photophysical properties and solvent effects. Chemical Physics Letters, 2016, 663, 45-50.	2.6	3
18	Conformational analysis of enantiomerization coupled to internal rotation in triptycyl-n-helicenes. Physical Chemistry Chemical Physics, 2019, 21, 11395-11404.	2.8	1

#	Article	IF	Citations
19	Theory of Exciton Dynamics in Thermally Activated Delayed Fluorescence. ChemPhotoChem, 2022, 6, .	3.0	1
20	Simple evaluation of dynamic disorder effects on exciton transport. Journal of Chemical Physics, 2022, 156, 044112.	3.0	0