J Martin Del Campo

List of Publications by Year
in descending order

28 papers	1,320 citations	687363 13 h-index	526287 27 g-index
29 all docs	29 docs citations	29 times ranked	1569 citing authors

#	Article	IF	Citations
1	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	3.0	425
2	Calculation of exchange-correlation potentials with auxiliary function densities. Journal of Chemical Physics, 2004, 121, 3417-3424.	3.0	190
3	deMon2k. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 548-555.	14.6	189
4	Experimental and Theoretical Study of the Structure and Reactivity of Fe_mO_n⁺ (m = 1, 2; n = 1â˜5) with CO. Journal of Physical Chemistry C, 2007, 111, 19086-19097.	3.1	81
5	Non-empirical improvement of PBE and its hybrid PBE0 for general description of molecular properties. Journal of Chemical Physics, 2012, 136, 104108.	3.0	78
6	A MinMax self-consistent-field approach for auxiliary density functional theory. Journal of Chemical Physics, 2009, 130, 114106.	3.0	59
7	A hierarchical transition state search algorithm. Journal of Chemical Physics, 2008, 129, 024107.	3.0	51
8	A new meta-GGA exchange functional based on an improved constraint-based GGA. Chemical Physics Letters, 2012, 543, 179-183.	2.6	44
9	Improved constraint satisfaction in a simple generalized gradient approximation exchange functional. Journal of Chemical Physics, 2012, 136, 144115.	3.0	31
10	Copper Coordination Features of Human Islet Amyloid Polypeptide: The Type 2 Diabetes Peptide. Inorganic Chemistry, 2016, 55, 10727-10740.	4.0	29
11	The reduced density gradient in atoms. International Journal of Quantum Chemistry, 2012, 112, 3594-3598.	2.0	27
12	Synthesis of Novel Chiral (Thio)ureas and Their Application as Organocatalysts and Ligands in Asymmetric Synthesis. Australian Journal of Chemistry, 2008, 61, 364.	0.9	17
13	A PW91-like exchange with a simple analytical form. Chemical Physics Letters, 2016, 651, 268-273.	2.6	16
14	Hybrid Functionals with Variationally Fitted Exact Exchange. Advances in Quantum Chemistry, 2015, 71, 41-67.	0.8	11
15	Resolution of the identity approximation applied to PNOF correlation calculations. Journal of Chemical Physics, 2021, 154, 064102.	3.0	11
16	Asmic: An Exceptional Building Block for Isocyanide Alkylations. Organic Letters, 2018, 20, 5910-5913.	4.6	9
17	Asmic Isocyanideâ€Nitrile Isomerizationâ€Alkylations. European Journal of Organic Chemistry, 2019, 2019, 4644-4648.	2.4	7
18	Asymmetric Density Fitting with Modified Cholesky Decomposition Applied to Second-Order Electron Propagator. Journal of Chemical Theory and Computation, 2020, 16, 1597-1605.	5.3	6

#	Article	IF	Citations
19	Self-Consistent Auxiliary Density Perturbation Theory. Journal of Chemical Theory and Computation, 2021, 17, 6934-6946.	5.3	6
20	Wettability of graphene oxide functionalized with N-alkylamines: a molecular dynamics study. Physical Chemistry Chemical Physics, 2022, 24, 11412-11419.	2.8	6
21	Theoretical analysis of the Sâ€“P bond in a family of compounds that involve a P2S2 ring: role of the PBE0-1/5 exchangeâ€“correlation functional. Computational and Theoretical Chemistry, 2015, 1062, 36-43.	2.5	5
22	Substrate Specificity and Leaving Group Effect in Ester Cleavage by Metal Complexes of an Oximate Nucleophile. Inorganic Chemistry, 2017, 56, 2060-2069.	4.0	5
23	Self-assembly and recognition properties of a tetraanionic macrocyclic boronate ester in aqueous medium. RSC Advances, 2015, 5, 30075-30083.	3.6	4
24	Theoretical study of the hydrogen bonding interaction between Levodopa and a new functionalized pillared coordination polymer designed as a carrier system. Journal of Molecular Structure, 2015, 1083, 106-110.	3.6	4
25	Understanding the unusual stiffness of hydrophobic dipeptide crystals. Physical Chemistry Chemical Physics, 2021, 23, 11931-11936.	2.8	4
26	Possible Use of Group 4 Metallocene Methyl Cations as Potential Neutralizers for FOX-7. Propellants, Explosives, Pyrotechnics, 2014, 39, 890-896.	1.6	3
27	B88 exchange functional recovering the local spin density linear response. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	2
28	- Local Virial Theorem for Ensembles of Excited States. , 2016, , 172-179.		0