Paula Mori-SÃ¡nchez

List of Publications by Year
in descending order

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29	14,453	218677	477307
papers	citations	26 h-index	29 g-index

29	29	29	13230
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Revealing Noncovalent Interactions. Journal of the American Chemical Society, 2010, 132, 6498-6506.	13.7	6,465
2	Insights into Current Limitations of Density Functional Theory. Science, 2008, 321, 792-794.	12.6	2,057
3	Challenges for Density Functional Theory. Chemical Reviews, 2012, 112, 289-320.	47.7	1,869
4	Localization and Delocalization Errors in Density Functional Theory and Implications for Band-Gap Prediction. Physical Review Letters, 2008, 100, 146401.	7.8	1,012
5	Many-electron self-interaction error in approximate density functionals. Journal of Chemical Physics, 2006, 125, 201102.	3.0	630
6	Development of exchange-correlation functionals with minimal many-electron self-interaction error. Journal of Chemical Physics, 2007, 126, 191109.	3.0	290
7	Fractional spins and static correlation error in density functional theory. Journal of Chemical Physics, 2008, 129, 121104.	3.0	215
8	Discontinuous Nature of the Exchange-Correlation Functional in Strongly Correlated Systems. Physical Review Letters, 2009, 102, 066403.	7.8	206
9	Self-interaction-free exchange-correlation functional for thermochemistry and kinetics. Journal of Chemical Physics, 2006, 124, 091102.	3.0	179
10	Pushing the frontiers of density functionals by solving the fractional electron problem. Science, 2021, 374, 1385-1389.	12.6	174
11	A Classification of Covalent, Ionic, and Metallic Solids Based on the Electron Density. Journal of the American Chemical Society, 2002, 124, 14721-14723.	13.7	160
12	Delocalization errors in density functionals and implications for main-group thermochemistry. Journal of Chemical Physics, 2008, 129, 204112.	3.0	159
13	Non-nuclear Maxima of the Electron Density. Physical Review Letters, 1999, 83, 1930-1933.	7.8	155
14	Accurate polymer polarizabilities with exact exchange density-functional theory. Journal of Chemical Physics, 2003, 119, 11001-11004.	3.0	154
15	Derivative discontinuity, bandgap and lowest unoccupied molecular orbital in density functional theory. Journal of Chemical Physics, 2012, 136, 204111.	3.0	154
16	Orbital-dependent correlation energy in density-functional theory based on a second-order perturbation approach: Success and failure. Journal of Chemical Physics, 2005, 123, 062204.	3.0	99
17	The derivative discontinuity of the exchangeâ€“correlation functional. Physical Chemistry Chemical Physics, 2014, 16, 14378-14387.	2.8	74
18	Second-Order Perturbation Theory with Fractional Charges and Fractional Spins. Journal of Chemical Theory and Computation, 2009, 5, 786-792.	5.3	61

#	Article	IF	Citations
19	Non-nuclear maxima of the electron density on alkaline metals. Journal of Chemical Physics, 2003, 119, 6341-6350.	3.0	54
20	Failure of the random-phase-approximation correlation energy. Physical Review A, 2012, 85, .	2.5	51
21	Fractional Charge Behavior and Band Gap Predictions with the XYG3 Type of Doubly Hybrid Density Functionals. Journal of Physical Chemistry A, 2014, 118, 9201-9211.	2.5	45
22	Ions in Crystals:â€‰ The Topology of the Electron Density in Ionic Materials. 4. The Danburite (CaB2Si2O8) Case and the Occurrence of Oxideâ''Oxide Bond Paths in Crystals. Journal of Physical Chemistry B, 2003, 107, 4912-4921.	2.6	36
23	Universal Features of the Topological Bond Properties of the Electron Density. Journal of Physical Chemistry A, 2004, 108, 2794-2801.	2.5	31
24	Extension of many-body theory and approximate density functionals to fractional charges and fractional spins. Journal of Chemical Physics, 2013, 139, 104114.	3.0	29
25	Landscape of an exact energy functional. Physical Review A, 2016, 93, .	2.5	27
26	Dramatic changes in electronic structure revealed by fractionally charged nuclei. Journal of Chemical Physics, 2014, 140, 044110.	3.0	26
27	Fermionic Statistics in the Strongly Correlated Limit of Density Functional Theory. Journal of Chemical Theory and Computation, 2017, 13, 6089-6100.	5.3	19
28	Exact Density Functional Obtained via the Levy Constrained Search. Journal of Physical Chemistry Letters, 2018, 9, 4910-4914.	4.6	13
29	Qualitative breakdown of the unrestricted Hartree-Fock energy. Journal of Chemical Physics, 2014, 141, 164124.	3.0	9