Juan I RodrÃ-guez

List of Publications by Year
in descending order

20	489	1040056 9	794594 19
papers	citations	h-index	g-index

20	20	20	496
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A high performance grid-based algorithm for computing QTAIM properties. Chemical Physics Letters, 2009, 472, 149-152.	2.6	151
2	An efficient method for computing the QTAIM topology of a scalar field: The electron density case. Journal of Computational Chemistry, 2013, 34, 681-686.	3.3	79
3	An efficient gridâ€based scheme to compute QTAIM atomic properties without explicit calculation of zeroâ€flux surfaces. Journal of Computational Chemistry, 2009, 30, 1082-1092.	3.3	73
4	Virial theorem in the Kohnâ€“Sham density-functional theory formalism: Accurate calculation of the atomic quantum theory of atoms in molecules energies. Journal of Chemical Physics, 2009, 131, 021101.	3.0	48
5	Numerical integration of exchange-correlation energies and potentials using transformed sparse grids. Journal of Chemical Physics, 2008, 128, 224103.	3.0	28
6	Structural and electronic properties of the P3HTâ€“PCBM dimer: A theoretical Study. Chemical Physics Letters, 2014, 612, 234-239.	2.6	17
7	Effects of Dispersion Forces on Structure and Photoinduced Charge Separation in Organic Photovoltaics. Journal of Physical Chemistry C, 2017, 121, 20134-20140.	3.1	14
8	Relativistic (SRâ€ZORA) quantum theory of atoms in molecules properties. Journal of Computational Chemistry, 2017, 38, 81-86.	3.3	12
9	Size evolution relativistic DFT-QTAIM study on the gold cluster complexes Au4-S-CnH2n-Sâ€²-Au4â€² (n =) Tj ETQq1 1 0.784314 rgBT	2.6	9
10	Molecular QTAIM Topology Is Sensitive to Relativistic Corrections. Chemistry - A European Journal, 2019, 25, 2538-2544.	3.3	9
11	A QTAIM topological analysis of the P3HTâ¿¿PCBM dimer. Chemical Physics Letters, 2016, 644, 157-162.	2.6	8
12	Insights into the all-metal [Sb3Au3Sb3]3â^' sandwich complex from a QTAIM and stress tensor analysis. Chemical Physics Letters, 2017, 685, 127-132.	2.6	8
13	Van der Waals effects on structure and optical properties in organic photovoltaics. International Journal of Quantum Chemistry, 2019, 119, e25883.	2.0	8
14	Size evolution study of â€œmolecularâ€•and â€œatom-in-clusterâ€•polarizabilities of medium-size gold clusters. Journal of Chemical Physics, 2011, 135, 034109.	3.0	7
15	Out of one, many â€” Using moment expansions of the virial relation to deduce universal density functionals from a single system. Canadian Journal of Chemistry, 2009, 87, 1540-1545.	1.1	6
16	Molecular (global) and atom-in-cluster (local) polarizabilities of medium-size gold nanoclusters: isomer structure effects. European Physical Journal D, 2013, 67, 1.	1.3	4
17	A size-selective method for increasing the performance of Pt supported on tungstated zirconia catalysts for alkane isomerization: a combined experimental and theoretical DFT study. New Journal of Chemistry, 2021, 45, 10510-10523.	2.8	4
18	Size evolution study on the electronic and optical properties of gold-cluster complexes <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si67.svg"><mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="italic">Au</mml:mi></mml:mrow><mml:mrow><mml:mn>4</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:m xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si68.svg"><mml:mrow><mml:msub><mml:mrow><mml:mi>C</mml:mi></mml:mrow><mml:mrow><mml:mi>n</mml:mi></mml:mrow></mml:mm	2.6	2

#	Article	IF	Citations
19	Unraveling the effects of Fe and Mn promoters on the tungstated zirconia catalyst: A DFT study. Applied Surface Science, 2022, 599, 154052.	6.1	2
20	Structure, Electronic, and Charge Transfer Properties of Organic Photovoltaics from Density Functional Theory Methods. Challenges and Advances in Computational Chemistry and Physics, 2021, , 57-79.	0.6	0