Alejandro F Maldonado

List of Publications by Year
in descending order

20	452	687363	794594
papers	citations	13	19
		h-index	g-index

20	20	20	173
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Microsolvation of Sr^{2+}, Ba^{2+}: Structures, energies, bonding, and nuclear magnetic shieldings. International Journal of Quantum Chemistry, 2021, 121, e26753.	2.0	7
2	Relativistic corrections of the electric field gradient in dihalogen molecules XY (X , Y Â=ÂF, Cl, Br, I, At) within the linear response elimination of the small component formalism. International Journal of Quantum Chemistry, 2021, 121, e26769.	2.0	1
3	Performance of the LRESC Model on top of DFT Functionals for Relativistic NMR Shielding Calculations. Journal of Chemical Information and Modeling, 2020, 60, 722-730.	5.4	7
4	Relativistic corrections to the electric field gradient given by linear response elimination of the small component formalism. International Journal of Quantum Chemistry, 2019, 119, e25935.	2.0	4
5	Theoretical developments and applications of polarization propagators. International Journal of Quantum Chemistry, 2019, 119, e25722.	2.0	17
6	Foundations of the LRESC model for response properties and some applications. International Journal of Quantum Chemistry, 2018, 118, e25487.	2.0	20
7	Microsolvation of methylmercury: structures, energies, bonding and NMR constants (^{199}Hg,^{13}C and^{17}O). Physical Chemistry Chemical Physics, 2016, 18, 1537-1550.	2.8	24
8	Absolute value of the nuclear magnetic shielding of silicon and germanium atoms in Si/Ge(CH3)4. Chemical Physics, 2015, 459, 125-130.	1.9	5
9	Theoretical analysis of NMR shieldings of group-11 metal halides on MX (M = Cu, Ag, Au; X = H, F, Cl, Br,) Tj ETQq1 1 0.784314 rgBT /O Physics, 2015, 17, 25516-25524.	2.8	12
10	Core-dependent and ligand-dependent relativistic corrections to the nuclear magnetic shieldings in MH4â^’n Y n (nâ‰=â‰0â€"4; M = Si, Ge, Sn, and Y = H, F, Cl, Br, I) model compounds. Journal of Molecular Modeling, 2014, 20, 2417.	1.8	23
11	Relativistic and Electron-Correlation Effects on the Nuclear Magnetic Resonance Shieldings of Molecules Containing Tin and Lead Atoms. Journal of Physical Chemistry A, 2014, 118, 7863-7875.	2.5	34
12	Nuclear charge-distribution effects on the NMR spectroscopy parameters. Journal of Chemical Physics, 2012, 136, 224110.	3.0	17
13	Relativistic effects on nuclear magnetic shieldings of $CH_nX4â^’n$ and CHXYZ (X, Y, Z = H, F,) Tj ETQq1 1 0.784314 rgBT /O	3.0	13
14	NMR espectroscopic parameters of HX and Si(Sn)X4 (X=H, F, Cl, Br and I) and SnBr4â^’nIn model compounds. Chemical Physics, 2012, 395, 75-81.	1.9	15
15	Relativistic effects on group-12 metal nuclear shieldings. Physical Chemistry Chemical Physics, 2011, 13, 21016.	2.8	35
16	Relativistic effects on the shielding of SnH2XY and PbH2XY (X, YÂ=ÂF, Cl, Br and I) heavy atomâ€"containing molecules. Theoretical Chemistry Accounts, 2011, 129, 483-494.	1.4	31
17	Polarization propagators: A powerful theoretical tool for a deeper understanding of NMR spectroscopic parameters. International Reviews in Physical Chemistry, 2010, 29, 1-64.	2.3	82
18	The UKB prescription and the heavy atom effects on the nuclear magnetic shielding of vicinal heavy atoms. Physical Chemistry Chemical Physics, 2009, 11, 5615.	2.8	67

#	Article	IF	Citations
19	The appearance of an interval of energies that contain the whole diamagnetic contribution to NMR magnetic shieldings. Journal of Chemical Physics, 2007, 127, 154115.	3.0	17
20	Relativistic effects on the nuclear magnetic shieldings of rare-gas atoms and halogen in hydrogen halides within relativistic polarization propagator theory. Journal of Chemical Physics, 2005, 123, 214108.	3.0	21