

Alejandro F Maldonado

List of Publications by Year in descending order

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papers

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687363

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794594

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all docs

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docs citations

20
times ranked

173
citing authors

#	ARTICLE	IF	CITATIONS
1	Polarization propagators: A powerful theoretical tool for a deeper understanding of NMR spectroscopic parameters. <i>International Reviews in Physical Chemistry</i> , 2010, 29, 1-64.	2.3	82
2	The UKB prescription and the heavy atom effects on the nuclear magnetic shielding of vicinal heavy atoms. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 5615.	2.8	67
3	Relativistic effects on group-12 metal nuclear shieldings. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 21016.	2.8	35
4	Relativistic and Electron-Correlation Effects on the Nuclear Magnetic Resonance Shieldings of Molecules Containing Tin and Lead Atoms. <i>Journal of Physical Chemistry A</i> , 2014, 118, 7863-7875.	2.5	34
5	Relativistic effects on the shielding of SnH ₂ XY and PbH ₂ XY (X, Y = F, Cl, Br and I) heavy atom-containing molecules. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 483-494.	1.4	31
6	Microsolvation of methylmercury: structures, energies, bonding and NMR constants (¹⁹⁹ Hg, ¹³ C and ¹⁷ O). <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 1537-1550.	2.8	24
7	Core-dependent and ligand-dependent relativistic corrections to the nuclear magnetic shieldings in MH ₄ Y _n (M = Si, Ge, Sn, and Y = H, F, Cl, Br, I) model compounds. <i>Journal of Molecular Modeling</i> , 2014, 20, 2417.	1.8	23
8	Relativistic effects on the nuclear magnetic shieldings of rare-gas atoms and halogen in hydrogen halides within relativistic polarization propagator theory. <i>Journal of Chemical Physics</i> , 2005, 123, 214108.	3.0	21
9	Foundations of the LRESC model for response properties and some applications. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25487.	2.0	20
10	The appearance of an interval of energies that contain the whole diamagnetic contribution to NMR magnetic shieldings. <i>Journal of Chemical Physics</i> , 2007, 127, 154115.	3.0	17
11	Nuclear charge-distribution effects on the NMR spectroscopy parameters. <i>Journal of Chemical Physics</i> , 2012, 136, 224110.	3.0	17
12	Theoretical developments and applications of polarization propagators. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25722.	2.0	17
13	NMR spectroscopic parameters of HX and Si(Sn)X ₄ (X=H, F, Cl, Br and I) and SnBr ₄ nIn model compounds. <i>Chemical Physics</i> , 2012, 395, 75-81.	1.9	15
14	Relativistic effects on nuclear magnetic shieldings of CH ₄ and CHXYZ (X, Y, Z = H, F, Cl, Br, I). <i>Journal of Chemical Physics</i> , 2007, 127, 154115.	3.0	13
15	Theoretical analysis of NMR shieldings of group-11 metal halides on MX (M = Cu, Ag, Au; X = H, F, Cl, Br, I). <i>Journal of Chemical Physics</i> , 2015, 143, 25516-25524.	2.8	12
16	Performance of the LRESC Model on top of DFT Functionals for Relativistic NMR Shielding Calculations. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 722-730.	5.4	7
17	Microsolvation of Sr ²⁺ , Ba ²⁺ : Structures, energies, bonding, and nuclear magnetic shieldings. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26753.	2.0	7
18	Absolute value of the nuclear magnetic shielding of silicon and germanium atoms in Si/Ge(CH ₃) ₄ . <i>Chemical Physics</i> , 2015, 459, 125-130.	1.9	5

#	ARTICLE	IF	CITATIONS
19	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
20	Relativistic corrections of the electric field gradient in dihalogen molecules XY (X, Y = F, 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