Gustavo A. Aucar

List of Publications by Year
in descending order

86	2,348	257101 24	233125 45
papers	citations	h-index	g-index

88	88	88	924
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Microsolvation of heavy halides. International Journal of Quantum Chemistry, 2021, 121, e26571.	1.0	13
2	Accurate location of hydrogen atoms in hydrogen bonds of tizoxanide from the combination of experimental and theoretical models. RSC Advances, 2021, 11, 7644-7652.	1.7	2
3	Microsolvation of Sr²⁺, Ba²⁺: Structures, energies, bonding, and nuclear magnetic shieldings. International Journal of Quantum Chemistry, 2021, 121, e26753.	1.0	7
4	Absolute NMR shielding scales in methyl halides obtained from experimental and calculated nuclear spin-rotation constants. Physical Review A, 2021, 104, .	1.0	4
5	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.	2.5	7
6	On the invariance of polarization propagators at SOPPA level of approach under unitary transformations of MOs. Chemical Physics Letters, 2020, 761, 138027.	1.2	0
7	On the quantum origin of few response properties. Journal of Chemical Physics, 2020, 153, 221101.	1.2	4
8	Magnetic descriptors of hydrogen bonds in malonaldehyde and its derivatives. Physical Chemistry Chemical Physics, 2019, 21, 19742-19754.	1.3	6
9	Relativistic and QED effects on NMR magnetic shielding constant of neutral and ionized atoms and diatomic molecules. Journal of Chemical Physics, 2019, 150, 184301.	1.2	15
10	Recent Developments in Absolute Shielding Scales for NMR Spectroscopy. Annual Reports on NMR Spectroscopy, 2019, 96, 77-141.	0.7	19
11	Theoretical developments and applications of polarization propagators. International Journal of Quantum Chemistry, 2019, 119, e25722.	1.0	17
12	QED effects on individual atomic orbital energies. Journal of Chemical Physics, 2018, 148, 134101.	1.2	15
13	Breit corrections to individual atomic and molecular orbital energies. Journal of Chemical Physics, 2018, 148, 044113.	1.2	16
14	Foundations of the LRESC model for response properties and some applications. International Journal of Quantum Chemistry, 2018, 118, e25487.	1.0	20
15	Polarization propagator theory and the entanglement between MO excitations. Physical Chemistry Chemical Physics, 2018, 20, 24832-24842.	1.3	3
16	Influence of the nuclear charge distribution and electron correlation effects on magnetic shieldings and spin-rotation tensors of linear molecules. RSC Advances, 2018, 8, 20234-20249.	1.7	6
17	Intermolecular magnetic interactions in stacked DNA base pairs. Physical Chemistry Chemical Physics, 2017, 19, 27817-27827.	1.3	5
18	Role of Spin-Dependent Terms in the Relationship among Nuclear Spin-Rotation and NMR Magnetic Shielding Tensors. Journal of Physical Chemistry Letters, 2016, 7, 5188-5192.	2.1	11

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19	Relativistic and electron correlation effects on NMR J-coupling of Sn and Pb containing molecules. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	16
20	Quantum electrodynamics effects on NMR magnetic shielding constants of He-like and Be-like atomic systems. Physical Review A, 2016, 93, .	1.0	11
21	Toward an absolute NMR shielding scale using the spin-rotation tensor within a relativistic framework. Physical Chemistry Chemical Physics, 2016, 18, 23572-23586.	1.3	11
22	Microsolvation of methylmercury: structures, energies, bonding and NMR constants (¹⁹⁹Hg,¹³C and¹⁷O). Physical Chemistry Chemical Physics, 2016, 18, 1537-1550.	1.3	24
23	Analysis of Proton NMR in Hydrogen Bonds in Terms of Loneâ€Pair and Bond Orbital Contributions. Chemistry - A European Journal, 2015, 21, 18138-18155.	1.7	19
24	Absolute value of the nuclear magnetic shielding of silicon and germanium atoms in Si/Ge(CH3)4. Chemical Physics, 2015, 459, 125-130.	0.9	5
25	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 /Ov Physics, 2015, 17, 25516-25524.	1.3	12
26	Toward a QFT-based theory of atomic and molecular properties. Physical Chemistry Chemical Physics, 2014, 16, 4420-4438.	1.3	26
27	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.	0.8	23
28	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.	1.1	34
29	Brief Account of Nonrelativistic Theory of NMR Parameters. Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems, 2013, , 9-39.	0.6	6
30	The Polarization Propagator Approach as a Tool to Study Electronic Molecular Structures from High-Resolution NMR Parameters. Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems, 2013, 3, 119-159.	0.6	5
31	The analysis of NMR J-couplings of saturated and unsaturated compounds by the localized second order polarization propagator approach method. Journal of Chemical Physics, 2012, 136, 174115.	1.2	6
32	Nuclear charge-distribution effects on the NMR spectroscopy parameters. Journal of Chemical Physics, 2012, 136, 224110.	1.2	17
33	Analysis of Electron Correlation Effects and Contributions of NMR J-Couplings from Occupied Localized Molecular Orbitals. Journal of Physical Chemistry A, 2012, 116, 1272-1282.	1.1	11
34	Relativistic effects on nuclear magnetic shieldings of CHnX4â^'n and CHXYZ (X, Y, Z = H, F,) Tj ETQq0 0 0 rgBT /Overlock 1	1.2	13
35	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.	0.9	15
36	Relativistic effects on group-12 metal nuclear shieldings. Physical Chemistry Chemical Physics, 2011, 13, 21016.	1.3	35

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37	Relativistic effects on the nuclear magnetic resonance shielding of FX (X = F, Cl, Br, I, and At) molecular systems. Journal of Chemical Physics, 2011, 134, 204314.	1.2	21
38	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.	0.5	31
39	Polarization propagators: A powerful theoretical tool for a deeper understanding of NMR spectroscopic parameters. International Reviews in Physical Chemistry, 2010, 29, 1-64.	0.9	82
40	NMR Spectroscopic Parameters of Molecular Systems with Strong Hydrogen Bonds. Journal of Physical Chemistry A, 2010, 114, 7162-7172.	1.1	32
41	The UKB prescription and the heavy atom effects on the nuclear magnetic shielding of vicinal heavy atoms. Physical Chemistry Chemical Physics, 2009, 11, 5615.	1.3	67
42	A computational study of ²J_{HH}(gem) indirect spinâ€“spin coupling constants in simple hydrides of the second and third periods. Magnetic Resonance in Chemistry, 2008, 46, 356-361.	1.1	16
43	Understanding NMR Jâ€couplings by the theory of polarization propagators. Concepts in Magnetic Resonance Part A: Bridging Education and Research, 2008, 32A, 88-116.	0.2	20
44	Theoretical NMR Spectroscopic Analysis of the Intramolecular Proton Transfer Mechanism in ortho-Hydroxyaryl (Un-)Substitued Schiff Bases. Journal of Physical Chemistry A, 2008, 112, 8767-8774.	1.1	13
45	The appearance of an interval of energies that contain the whole diamagnetic contribution to NMR magnetic shieldings. Journal of Chemical Physics, 2007, 127, 154115.	1.2	17
46	Relativistic heavy-atom effects on heavy-atom nuclear shieldings. Journal of Chemical Physics, 2006, 125, 184113.	1.2	48
47	On the Usage of Locally Dense Basis Sets in the Calculation of NMR Indirect Nuclear Spinâ€“Spin Coupling Constants: Vicinal Fluorineâ€“Fluorine Couplings. Advances in Quantum Chemistry, 2005, , 161-183.	0.4	65
48	Relativistic corrections to the diamagnetic term of the nuclear magnetic shielding: Analysis of contributions from localized orbitals. Journal of Chemical Physics, 2005, 122, 064103.	1.2	18
49	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.	1.2	21
50	Theoretical Study of HCN and HNC Neutral and Charged Clusters. Journal of Physical Chemistry B, 2005, 109, 18189-18194.	1.2	55
51	Interaction Energies and NMR Indirect Nuclear Spinâ^'Spin Coupling Constants in Linear HCN and HNC Complexes. Journal of Physical Chemistry A, 2005, 109, 6555-6564.	1.1	52
52	Relativistic effects on nuclear magnetic shielding constants in HX and CH3Xâ€Š(X=Br,I) based on the linear response within the elimination of small component approach. Journal of Chemical Physics, 2004, 121, 6798-6808.	1.2	71
53	Hyperconjugation:Â The Electronic Mechanism That May Underlie the Karplus Curve of Vicinal NMR Indirect Spin Couplings. Journal of Physical Chemistry A, 2004, 108, 6231-6238.	1.1	11
54	Large Long-Range Fâ^'F Indirect Spinâ^'Spin Coupling Constants. Prediction of Measurable Fâ^'F Couplings over a Few Nanometers. Journal of Physical Chemistry A, 2004, 108, 5393-5398.	1.1	49

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55	Relativistic mass-corrections to the heavy atom nuclear magnetic shieldings. Analysis of contributions in terms of localized orbitals. Chemical Physics Letters, 2003, 367, 265-269.	1.2	20
56	Propagator matrices as matrices of power's series. II. It's relationship with HF's stability problem and alternative solutions. Computational and Theoretical Chemistry, 2003, 620, 149-156.	1.5	8
57	Relativistic effects on the nuclear magnetic shielding tensor. Journal of Chemical Physics, 2003, 118, 471-486.	1.2	86
58	The Effect of Substituents on Indirect Nuclear Spin-Spin Coupling Constants: Methan- and Ethanimine, Methanal- and Ethanaloxime. International Journal of Molecular Sciences, 2003, 4, 231-248.	1.8	24
59	QED approach to the nuclear spin-spin coupling tensor. Physical Review A, 2002, 65, .	1.0	24
60	Fully relativistic calculation of nuclear magnetic shieldings and indirect nuclear spin-spin couplings in group-15 and -16 hydrides. Journal of Chemical Physics, 2002, 117, 7942-7946.	1.2	60
61	Self-energy Effects on Nuclear Magnetic Resonance Parameters within Quantum Electrodynamics Perturbation Theory. International Journal of Molecular Sciences, 2002, 3, 914-930.	1.8	17
62	Propagator matrices as matrices of power's series. I. Its zeroth-order and the Popleâ€“Santry model. Computational and Theoretical Chemistry, 2002, 584, 159-168.	1.5	9
63	The effect of lone pairs and electronegativity on the indirect nuclear spinâ€“spin coupling constants in CH2X (X=CH2, NH, O, S):Ab initiocalculations using optimized contracted basis sets. Journal of Chemical Physics, 2001, 115, 1324-1334.	1.2	252
64	Implementation of the IPPPâ€“CLOPPAâ€“INDO/S method for the study of indirect nuclear spin coupling constants and its application to molecules containing tin nuclei. Journal of Organometallic Chemistry, 2000, 598, 193-201.	0.8	6
65	The use of locally dense basis sets in the calculation of indirect nuclear spinâ€“spin coupling constants: The vicinal coupling constants in H3Câ€“CH2X (X=H, F, Cl, Br, I). Journal of Chemical Physics, 2000, 112, 6201-6208.	1.2	86
66	Reply to â€œComment on â€˜Relativistic correction of the generalized oscillator strength sum rulesâ€™ â€: Physical Review A, 1999, 59, 4849-4849.	1.0	0
67	On the origin and contribution of the diamagnetic term in four-component relativistic calculations of magnetic properties. Journal of Chemical Physics, 1999, 110, 6208-6218.	1.2	198
68	NMR-K reduced coupling constant calculations within the CLOPPA-PM3 approach: I. General results. Computational and Theoretical Chemistry, 1998, 452, 1-11.	1.5	15
69	NMR-K reduced coupling constants within the CLOPPA-PM3 approach. II: shortcomings and how to overcome them. Computational and Theoretical Chemistry, 1998, 452, 13-23.	1.5	17
70	Relativistic correction of the generalized oscillator strength sum rules. Physical Review A, 1998, 57, 2212-2215.	1.0	7
71	Experimental and theoretical study of substituent effects on3J(13C1-1H) coupling constants in 1-X-bicyclo[1.1.1]pentanes. Journal of Physical Organic Chemistry, 1996, 9, 168-178.	0.9	20
72	Restrictions on ground state average values imposed by time reversal symmetry. Chemical Physics Letters, 1996, 254, 13-20.	1.2	3

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73	RPA AM1 calculations of NMR spin-spin coupling constants: geminal119Sn119Sn couplings. Journal of Organometallic Chemistry, 1996, 524, 1-7.	0.8	17
74	Operator representations in Kramers bases. Chemical Physics Letters, 1995, 232, 47-53.	1.2	27
75	RPA MNDO analysis of the dihedral angle dependence of vicinal J(SnSn) and J(SnC) NMR coupling constants. Computational and Theoretical Chemistry, 1995, 330, 211-216.	1.5	6
76	Relativistic extension of the Bethe sum rule. Physical Review A, 1995, 52, 1054-1059.	1.0	15
77	Polarization propagator analysis of the through space transmission of spinâ€"spin coupling constants by overlap of lone pairs. Journal of Molecular Structure, 1993, 300, 467-477.	1.8	13
78	Relativistic theory for indirect nuclear spin-spin couplings within the polarization propagator approach. International Journal of Quantum Chemistry, 1993, 47, 425-435.	1.0	101
79	Viewpoint 8 â€" polarization propagator analysis of spin-spin coupling constants. Computational and Theoretical Chemistry, 1993, 284, 249-269.	1.5	60
80	New method to study spin-spin coupling constants involving heavy nuclei at the MNDO-RPA level with localized orbitals. Journal of Magnetic Resonance, 1991, 93, 413-418.	0.5	13
81	Quantum chemical analysis of the orientational lone-pair effect on spin-spin coupling constants. Computational and Theoretical Chemistry, 1990, 210, 175-186.	1.5	30
82	Large spin-dipolar long-range F-F coupling constants in conjugative compounds: their study using propagators. Computational and Theoretical Chemistry, 1990, 210, 205-210.	1.5	13
83	Analysis of multipath transmission of spin-spin coupling constants in 1-x-bicycloalkanes. Computational and Theoretical Chemistry, 1990, 205, 79-88.	1.5	25
84	Analysis of the phosphorus lone-pair orientational effect on 31Pî—¸13C couplings in 7-(phosphamethyl)norbornene. Computational and Theoretical Chemistry, 1988, 164, 1-15.	1.5	13
85	Theoretical IPPP analysis of13C-31 P through-space indirect couplings in phosphorus-substituted alkenes. Magnetic Resonance in Chemistry, 1987, 25, 883-888.	1.1	13
86	Relativistic and QED corrections to one-bond indirect nuclear spin-spin couplings in X$_2^{2+}$ and X$_3^{2+}$ ions (X = Zn, Cd, Hg). Journal of Chemical Physics, 0, , .	1.2	2