

Gustavo A. Aucar

List of Publications by Year in descending order

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86
papers

2,348
citations

257101

24
h-index

233125

45
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88
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88
docs citations

88
times ranked

924
citing authors

#	ARTICLE	IF	CITATIONS
1	The effect of lone pairs and electronegativity on the indirect nuclear spin-spin coupling constants in CH ₂ X (X=CH ₂ , NH, O, S): Ab initio calculations using optimized contracted basis sets. <i>Journal of Chemical Physics</i> , 2001, 115, 1324-1334.	1.2	252
2	On the origin and contribution of the diamagnetic term in four-component relativistic calculations of magnetic properties. <i>Journal of Chemical Physics</i> , 1999, 110, 6208-6218.	1.2	198
3	Relativistic theory for indirect nuclear spin-spin couplings within the polarization propagator approach. <i>International Journal of Quantum Chemistry</i> , 1993, 47, 425-435.	1.0	101
4	The use of locally dense basis sets in the calculation of indirect nuclear spin-spin coupling constants: The vicinal coupling constants in H ₃ C-CH ₂ X (X=H, F, Cl, Br, I). <i>Journal of Chemical Physics</i> , 2000, 112, 6201-6208.	1.2	86
5	Relativistic effects on the nuclear magnetic shielding tensor. <i>Journal of Chemical Physics</i> , 2003, 118, 471-486.	1.2	86
6	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.	0.9	82
7	Relativistic effects on nuclear magnetic shielding constants in HX and CH ₃ X (X=Br, I) based on the linear response within the elimination of small component approach. <i>Journal of Chemical Physics</i> , 2004, 121, 6798-6808.	1.2	71
8	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.	1.3	67
9	On the Usage of Locally Dense Basis Sets in the Calculation of NMR Indirect Nuclear Spin-Spin Coupling Constants: Vicinal Fluorine-Fluorine Couplings. <i>Advances in Quantum Chemistry</i> , 2005, , 161-183.	0.4	65
10	Viewpoint 8 - polarization propagator analysis of spin-spin coupling constants. <i>Computational and Theoretical Chemistry</i> , 1993, 284, 249-269.	1.5	60
11	Fully relativistic calculation of nuclear magnetic shieldings and indirect nuclear spin-spin couplings in group-15 and -16 hydrides. <i>Journal of Chemical Physics</i> , 2002, 117, 7942-7946.	1.2	60
12	Theoretical Study of HCN and HNC Neutral and Charged Clusters. <i>Journal of Physical Chemistry B</i> , 2005, 109, 18189-18194.	1.2	55
13	Interaction Energies and NMR Indirect Nuclear Spin-Spin Coupling Constants in Linear HCN and HNC Complexes. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6555-6564.	1.1	52
14	Large Long-Range F-F Indirect Spin-Spin Coupling Constants. Prediction of Measurable F-F Couplings over a Few Nanometers. <i>Journal of Physical Chemistry A</i> , 2004, 108, 5393-5398.	1.1	49
15	Relativistic heavy-atom effects on heavy-atom nuclear shieldings. <i>Journal of Chemical Physics</i> , 2006, 125, 184113.	1.2	48
16	Relativistic effects on group-12 metal nuclear shieldings. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 21016.	1.3	35
17	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.	1.1	34
18	NMR Spectroscopic Parameters of Molecular Systems with Strong Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7162-7172.	1.1	32

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19	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.	0.5	31
20	Quantum chemical analysis of the orientational lone-pair effect on spin-spin coupling constants. <i>Computational and Theoretical Chemistry</i> , 1990, 210, 175-186.	1.5	30
21	Operator representations in Kramers bases. <i>Chemical Physics Letters</i> , 1995, 232, 47-53.	1.2	27
22	Toward a QFT-based theory of atomic and molecular properties. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 4420-4438.	1.3	26
23	Analysis of multipath transmission of spin-spin coupling constants in 1-x-bicycloalkanes. <i>Computational and Theoretical Chemistry</i> , 1990, 205, 79-88.	1.5	25
24	QED approach to the nuclear spin-spin coupling tensor. <i>Physical Review A</i> , 2002, 65, .	1.0	24
25	The Effect of Substituents on Indirect Nuclear Spin-Spin Coupling Constants: Methan- and Ethanimine, Methanal- and Ethanaloxime. <i>International Journal of Molecular Sciences</i> , 2003, 4, 231-248.	1.8	24
26	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.	1.3	24
27	Core-dependent and ligand-dependent relativistic corrections to the nuclear magnetic shieldings in MH ₄ Y _n (n = 4; M = Si, Ge, Sn, and Y = H, F, Cl, Br, I) model compounds. <i>Journal of Molecular Modeling</i> , 2014, 20, 2417.	0.8	23
28	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.	1.2	21
29	Relativistic effects on the nuclear magnetic resonance shielding of FX (X = F, Cl, Br, I, and At) molecular systems. <i>Journal of Chemical Physics</i> , 2011, 134, 204314.	1.2	21
30	Experimental and theoretical study of substituent effects on ³ J(¹³ C- ¹ H) coupling constants in 1-X-bicyclo[1.1.1]pentanes. <i>Journal of Physical Organic Chemistry</i> , 1996, 9, 168-178.	0.9	20
31	Relativistic mass-corrections to the heavy atom nuclear magnetic shieldings. Analysis of contributions in terms of localized orbitals. <i>Chemical Physics Letters</i> , 2003, 367, 265-269.	1.2	20
32	Understanding NMR couplings by the theory of polarization propagators. <i>Concepts in Magnetic Resonance Part A: Bridging Education and Research</i> , 2008, 32A, 88-116.	0.2	20
33	Foundations of the LRESC model for response properties and some applications. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25487.	1.0	20
34	Analysis of Proton NMR in Hydrogen Bonds in Terms of Lone-Pair and Bond Orbital Contributions. <i>Chemistry - A European Journal</i> , 2015, 21, 18138-18155.	1.7	19
35	Recent Developments in Absolute Shielding Scales for NMR Spectroscopy. <i>Annual Reports on NMR Spectroscopy</i> , 2019, 96, 77-141.	0.7	19
36	Relativistic corrections to the diamagnetic term of the nuclear magnetic shielding: Analysis of contributions from localized orbitals. <i>Journal of Chemical Physics</i> , 2005, 122, 064103.	1.2	18

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37	RPA AM1 calculations of NMR spin-spin coupling constants: geminal ^{119}Sn - ^{119}Sn couplings. <i>Journal of Organometallic Chemistry</i> , 1996, 524, 1-7.	0.8	17
38	NMR-K reduced coupling constants within the CLOPPA-PM3 approach. II: shortcomings and how to overcome them. <i>Computational and Theoretical Chemistry</i> , 1998, 452, 13-23.	1.5	17
39	Self-energy Effects on Nuclear Magnetic Resonance Parameters within Quantum Electrodynamics Perturbation Theory. <i>International Journal of Molecular Sciences</i> , 2002, 3, 914-930.	1.8	17
40	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.	1.2	17
41	Nuclear charge-distribution effects on the NMR spectroscopy parameters. <i>Journal of Chemical Physics</i> , 2012, 136, 224110.	1.2	17
42	Theoretical developments and applications of polarization propagators. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25722.	1.0	17
43	A computational study of $\langle \sup>2</sup> \langle i \rangle J \langle /i \rangle \langle \sub>HH</sub> \langle i \rangle \text{gem} \langle /i \rangle$ indirect spin-spin coupling constants in simple hydrides of the second and third periods. <i>Magnetic Resonance in Chemistry</i> , 2008, 46, 356-361.	1.1	16
44	Relativistic and electron correlation effects on NMR J-coupling of Sn and Pb containing molecules. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	16
45	Breit corrections to individual atomic and molecular orbital energies. <i>Journal of Chemical Physics</i> , 2018, 148, 044113.	1.2	16
46	Relativistic extension of the Bethe sum rule. <i>Physical Review A</i> , 1995, 52, 1054-1059.	1.0	15
47	NMR-K reduced coupling constant calculations within the CLOPPA-PM3 approach: I. General results. <i>Computational and Theoretical Chemistry</i> , 1998, 452, 1-11.	1.5	15
48	NMR spectroscopic parameters of HX and $\text{Si}(\text{Sn})\text{X}_4$ ($\text{X}=\text{H}, \text{F}, \text{Cl}, \text{Br}$ and I) and $\text{SnBr}_4 \cdot n\text{In}$ model compounds. <i>Chemical Physics</i> , 2012, 395, 75-81.	0.9	15
49	QED effects on individual atomic orbital energies. <i>Journal of Chemical Physics</i> , 2018, 148, 134101.	1.2	15
50	Relativistic and QED effects on NMR magnetic shielding constant of neutral and ionized atoms and diatomic molecules. <i>Journal of Chemical Physics</i> , 2019, 150, 184301.	1.2	15
51	Theoretical IPPP analysis of ^{13}C - ^{31}P through-space indirect couplings in phosphorus-substituted alkenes. <i>Magnetic Resonance in Chemistry</i> , 1987, 25, 883-888.	1.1	13
52	Analysis of the phosphorus lone-pair orientational effect on ^{31}P - ^{13}C couplings in 7-(phosphamethyl)norborene. <i>Computational and Theoretical Chemistry</i> , 1988, 164, 1-15.	1.5	13
53	Large spin-dipolar long-range F-F coupling constants in conjugative compounds: their study using propagators. <i>Computational and Theoretical Chemistry</i> , 1990, 210, 205-210.	1.5	13
54	New method to study spin-spin coupling constants involving heavy nuclei at the MNDO-RPA level with localized orbitals. <i>Journal of Magnetic Resonance</i> , 1991, 93, 413-418.	0.5	13

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55	Polarization propagator analysis of the through space transmission of spin-spin coupling constants by overlap of lone pairs. <i>Journal of Molecular Structure</i> , 1993, 300, 467-477.	1.8	13
56	Theoretical NMR Spectroscopic Analysis of the Intramolecular Proton Transfer Mechanism in <i>o</i> -Hydroxyaryl (Un-)Substituted Schiff Bases. <i>Journal of Physical Chemistry A</i> , 2008, 112, 8767-8774.	1.1	13
57	Relativistic effects on nuclear magnetic shieldings of CH_4 and CHXYZ (X, Y, Z = H, F). <i>J. Chem. Phys.</i> 112, 10784 (2000).	1.2	13
58	Microsolvation of heavy halides. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26571.	1.0	13
59	Theoretical analysis of NMR shieldings of group-11 metal halides on MX (M = Cu, Ag, Au; X = H, F, Cl, Br). <i>J. Chem. Phys.</i> 123, 25516 (2005).	1.3	12
60	Hyperconjugation: The Electronic Mechanism That May Underlie the Karplus Curve of Vicinal NMR Indirect Spin Couplings. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6231-6238.	1.1	11
61	Analysis of Electron Correlation Effects and Contributions of NMR J-Couplings from Occupied Localized Molecular Orbitals. <i>Journal of Physical Chemistry A</i> , 2012, 116, 1272-1282.	1.1	11
62	Role of Spin-Dependent Terms in the Relationship among Nuclear Spin-Rotation and NMR Magnetic Shielding Tensors. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 5188-5192.	2.1	11
63	Quantum electrodynamics effects on NMR magnetic shielding constants of He-like and Be-like atomic systems. <i>Physical Review A</i> , 2016, 93, .	1.0	11
64	Toward an absolute NMR shielding scale using the spin-rotation tensor within a relativistic framework. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 23572-23586.	1.3	11
65	Propagator matrices as matrices of power's series. I. Its zeroth-order and the Pople's Santry model. <i>Computational and Theoretical Chemistry</i> , 2002, 584, 159-168.	1.5	9
66	Propagator matrices as matrices of power's series. II. Its relationship with HF's stability problem and alternative solutions. <i>Computational and Theoretical Chemistry</i> , 2003, 620, 149-156.	1.5	8
67	Relativistic correction of the generalized oscillator strength sum rules. <i>Physical Review A</i> , 1998, 57, 2212-2215.	1.0	7
68	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.	2.5	7
69	Microsolvation of Sr^{2+} , Ba^{2+} : Structures, energies, bonding, and nuclear magnetic shieldings. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26753.	1.0	7
70	RPA MNDO analysis of the dihedral angle dependence of vicinal $J(\text{SnSn})$ and $J(\text{SnC})$ NMR coupling constants. <i>Computational and Theoretical Chemistry</i> , 1995, 330, 211-216.	1.5	6
71	Implementation of the IPPP's CLOPPA's INDO/S method for the study of indirect nuclear spin coupling constants and its application to molecules containing tin nuclei. <i>Journal of Organometallic Chemistry</i> , 2000, 598, 193-201.	0.8	6
72	The analysis of NMR J-couplings of saturated and unsaturated compounds by the localized second order polarization propagator approach method. <i>Journal of Chemical Physics</i> , 2012, 136, 174115.	1.2	6

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73	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
74	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
75	Magnetic descriptors of hydrogen bonds in malonaldehyde and its derivatives. Physical Chemistry Chemical Physics, 2019, 21, 19742-19754.	1.3	6
76	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
77	Absolute value of the nuclear magnetic shielding of silicon and germanium atoms in Si/Ge(CH ₃) ₄ . Chemical Physics, 2015, 459, 125-130.	0.9	5
78	Intermolecular magnetic interactions in stacked DNA base pairs. Physical Chemistry Chemical Physics, 2017, 19, 27817-27827.	1.3	5
79	On the quantum origin of few response properties. Journal of Chemical Physics, 2020, 153, 221101.	1.2	4
80	Absolute NMR shielding scales in methyl halides obtained from experimental and calculated nuclear spin-rotation constants. Physical Review A, 2021, 104, .	1.0	4
81	Restrictions on ground state average values imposed by time reversal symmetry. Chemical Physics Letters, 1996, 254, 13-20.	1.2	3
82	Polarization propagator theory and the entanglement between MO excitations. Physical Chemistry Chemical Physics, 2018, 20, 24832-24842.	1.3	3
83	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
84	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
85	Reply to "Comment on "Relativistic correction of the generalized oscillator strength sum rules"â€™. Physical Review A, 1999, 59, 4849-4849.	1.0	0
86	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