

# Alfredo M Simas

## List of Publications by Year in descending order

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114  
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5,204  
citations

147801

31  
h-index

91884

69  
g-index

115  
all docs

115  
docs citations

115  
times ranked

4072  
citing authors

#	ARTICLE	IF	CITATIONS
1	Spectroscopic properties and design of highly luminescent lanthanide coordination complexes. <i>Coordination Chemistry Reviews</i> , 2000, 196, 165-195.	18.8	1,417
2	RM1: A reparameterization of AM1 for H, C, N, O, P, S, F, Cl, Br, and I. <i>Journal of Computational Chemistry</i> , 2006, 27, 1101-1111.	3.3	634
3	Sparkle Model for the Calculation of Lanthanide Complexes: AM1 Parameters for Eu(III), Gd(III), and Tb(III). <i>Inorganic Chemistry</i> , 2005, 44, 3299-3310.	4.0	133
4	The Laplacian of the charge density and its relationship to the shell structure of atoms and ions. <i>Journal of Chemical Physics</i> , 1988, 88, 4367-4374.	3.0	132
5	Sparkle model for the quantum chemical AM1 calculation of europium complexes. <i>Chemical Physics Letters</i> , 1994, 227, 349-353.	2.6	128
6	Synthesis, X-ray Structure, Spectroscopic Characterization, and Theoretical Prediction of the Structure and Electronic Spectrum of Eu(btfa) <sub>3</sub> ·bipy and an Assessment of the Effect of Fluorine as a $\beta^2$ -Diketone Substituent on the Ligand-Metal Energy Transfer Process. <i>Inorganic Chemistry</i> , 1998, 37, 3542-3547.	4.0	113
7	Sparkle/PM7 Lanthanide Parameters for the Modeling of Complexes and Materials. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3333-3341.	5.3	107
8	Importance of Tautomers in the Chemical Behavior of Tetracyclines. <i>Journal of Pharmaceutical Sciences</i> , 1999, 88, 111-120.	3.3	105
9	A Comprehensive Strategy to Boost the Quantum Yield of Luminescence of Europium Complexes. <i>Scientific Reports</i> , 2013, 3, 2395.	3.3	101
10	Photoluminescence of Europium(III) Dithiocarbamate Complexes: Electronic Structure, Charge Transfer and Energy Transfer. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2510-2516.	2.5	98
11	Sparkle/PM6 Parameters for all Lanthanide Trications from La(III) to Lu(III). <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2019-2023.	5.3	84
12	Internally folded densities. <i>Chemical Physics</i> , 1981, 63, 175-183.	1.9	69
13	Sparkle Model for AM1 Calculation of Lanthanide Complexes: Improved Parameters for Europium. <i>Inorganic Chemistry</i> , 2004, 43, 2346-2354.	4.0	65
14	Sparkle/PM3 for the modeling of europium(III), gadolinium(III), and terbium(III) complexes. <i>Journal of the Brazilian Chemical Society</i> , 2009, 20, 1638-1645.	0.6	59
15	Theoretical model for the prediction of electronic spectra of lanthanide complexes. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1996, 92, 1835-1839.	1.7	58
16	Sparkle/RM1 parameters for the semiempirical quantum chemical calculation of lanthanide complexes. <i>RSC Advances</i> , 2013, 3, 16747.	3.6	58
17	Lanthanide complex coordination polyhedron geometry prediction accuracies of ab initio effective core potential calculations. <i>Journal of Molecular Modeling</i> , 2006, 12, 373-389.	1.8	56
18	Basis set quality. II. Information theoretic appraisal of various orbitals. <i>International Journal of Quantum Chemistry</i> , 1983, 24, 527-550.	2.0	54

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19	Momentum space properties of various orbital basis sets used in quantum chemical calculations. <i>International Journal of Quantum Chemistry</i> , 1982, 21, 419-429.	2.0	51
20	Mesoionic rings as efficient asymmetric bridges for the design of compounds with large optical nonlinearities. <i>Chemical Physics Letters</i> , 1996, 257, 639-646.	2.6	50
21	Hepatitis C virus infection diagnosis using metabonomics. <i>Journal of Viral Hepatitis</i> , 2010, 17, 854-858.	2.0	47
22	On the applicability of CNDO indices for the prediction of chemical reactivity. <i>Theoretica Chimica Acta</i> , 1982, 62, 1-16.	0.8	45
23	The nonmonotonic behavior of and the presence of slow and fast maxima in the momentum densities of atoms and ions. <i>Journal of Chemical Physics</i> , 1985, 83, 4054-4058.	3.0	45
24	Sparkle model for the quantum chemical AM1 calculation of europium complexes of coordination number nine. <i>Journal of Alloys and Compounds</i> , 1995, 225, 55-59.	5.5	43
25	Extraction of momentum expectation values from Compton profiles. <i>Molecular Physics</i> , 1980, 41, 1153-1162.	1.7	42
26	Sparkle/AM1 Parameters for the Modeling of Samarium(III) and Promethium(III) Complexes. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 64-74.	5.3	37
27	Modeling rare earth complexes: Sparkle/PM3 parameters for thulium(III). <i>Chemical Physics Letters</i> , 2006, 425, 138-141.	2.6	36
28	RM1 Model for the Prediction of Geometries of Complexes of the Trications of Eu, Gd, and Tb. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3031-3037.	5.3	36
29	Reaction-field "supermolecule approach to calculation of solvent effects. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1992, 88, 189-193.	1.7	34
30	Europium Luminescence: Electronic Densities and Superdelocalizabilities for a Unique Adjustment of Theoretical Intensity Parameters. <i>Scientific Reports</i> , 2015, 5, 13695.	3.3	33
31	The shell structure of atoms and ions in momentum space. <i>Journal of Chemical Physics</i> , 1984, 80, 2636-2642.	3.0	32
32	Efficacy of the semiempirical sparkle model as compared to ECP ab-initio calculations for the prediction of ligand field parameters of europium (III) complexes. <i>Journal of Luminescence</i> , 2005, 111, 81-87.	3.1	32
33	Synthesis and Antiinflammatory Activity of 3-Aryl-5-Isopropyl-1,2,4-Oxadiazoles. <i>Heterocyclic Communications</i> , 2000, 6, .	1.2	31
34	MESOIONIC 2-N-CYCLOALKYLAMINO-5-ALKYL-1,3-DITHIOLIUM-4-THIOLATES. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 1996, 108, 75-84.	1.6	30
35	Design of ligands to obtain lanthanide ion complexes displaying high quantum efficiencies of luminescence using the sparkle model. <i>Computational and Theoretical Chemistry</i> , 2000, 527, 245-251.	1.5	30
36	Antinociceptive pyrimidine derivatives: aqueous multicomponent microwave assisted synthesis. <i>Tetrahedron Letters</i> , 2013, 54, 3462-3465.	1.4	29

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37	Sparkle/AM1 Structure Modeling of Lanthanum (III) and Lutetium (III) Complexes. <i>Journal of Physical Chemistry A</i> , 2006, 110, 5897-5900.	2.5	28
38	Partial wave analysis of the momentum density. <i>Journal of Chemical Physics</i> , 1984, 81, 2953-2961.	3.0	27
39	Sparkle/PM3 Parameters for the Modeling of Neodymium(III), Promethium(III), and Samarium(III) Complexes. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1588-1596.	5.3	27
40	Topographical features of the Laplacian of the momentum density of atoms and ions most indicative of shell structure. <i>Journal of Chemical Physics</i> , 1989, 90, 6520-6527.	3.0	26
41	Modeling Lanthanide Complexes: Towards the Theoretical Design of Light Conversion Molecular Devices. <i>Molecular Engineering</i> , 1997, 7, 293-308.	0.2	26
42	Are mesoionic compounds aromatic?. <i>Canadian Journal of Chemistry</i> , 1998, 76, 869-872.	1.1	26
43	The generator coordinate Hartree-Fock method for molecular systems. Formalism and first applications to H <sub>2</sub> , LiH and Li <sub>2</sub> . <i>Chemical Physics</i> , 1991, 154, 379-384.	1.9	25
44	The generator coordinate Hartree-Fock method for molecular systems. Near Hartree-Fock limit calculations for N <sub>2</sub> , CO and BF. <i>Chemical Physics Letters</i> , 1992, 192, 195-198.	2.6	24
45	Two-photon absorption in mesoionic compounds pumped at the visible and at the infrared. <i>Chemical Physics Letters</i> , 2000, 332, 13-18.	2.6	24
46	Chemical Partition of the Radiative Decay Rate of Luminescence of Europium Complexes. <i>Scientific Reports</i> , 2016, 6, 21204.	3.3	24
47	Europium Complexes: Luminescence Boost by a Single Efficient Antenna Ligand. <i>ACS Omega</i> , 2017, 2, 6786-6794.	3.5	24
48	Efficient Chiral Discrimination by <sup>77</sup> Se NMR. <i>Organic Letters</i> , 2003, 5, 1601-1604.	4.6	23
49	Sparkle model for AM1 calculation of neodymium(III) coordination compounds. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2006, 177, 225-237.	3.9	23
50	Structure Modeling of Trivalent Lanthanum and Lutetium Complexes: Sparkle/PM3. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5015-5018.	2.5	23
51	Exact topological twistons in crystalline polyethylene. <i>Chemical Physics Letters</i> , 2000, 320, 587-593.	2.6	22
52	AM1 Sparkle modeling of Er(III) and Ce(III) coordination compounds. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 2584-2588.	1.8	22
53	Lanthanide coordination compounds modeling: Sparkle/PM3 parameters for dysprosium (III), holmium (III) and erbium (III). <i>Journal of Organometallic Chemistry</i> , 2008, 693, 1952-1956.	1.8	22
54	Two-Photon Absorption by Fluorene Derivatives: Systematic Molecular Design. <i>Journal of Physical Chemistry C</i> , 2010, 114, 6106-6116.	3.1	21

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55	Excited state calculations of Europium(III) complexes. <i>Journal of Alloys and Compounds</i> , 1997, 250, 412-416.	5.5	20
56	Synthesis, crystal structure determination and theoretical prediction of the structure and electronic spectrum of Eu(btfa) <sub>3</sub> bipy. <i>Journal of Luminescence</i> , 1997, 72-74, 159-161.	3.1	19
57	Mesoionic rings as third-order non-linear optical materials. <i>Chemical Physics Letters</i> , 1999, 309, 421-426.	2.6	19
58	Nonlinear absorption of new mesoionic compounds. <i>Optics Communications</i> , 2006, 264, 225-228.	2.1	19
59	Synthesis and Characterization of some New Mesoionic 1,3-Thiazolium-5-thiolates via Cyclodehydration and in situ 1,3-Dipolar Cycloaddition/Cycloreversion. <i>Molecules</i> , 2002, 7, 791-800.	3.8	19
60	Modeling lanthanide complexes: Sparkle/AM1 parameters for ytterbium (III). <i>Journal of Computational Chemistry</i> , 2005, 26, 1524-1528.	3.3	18
61	Sparkle/PM3 parameters for praseodymium(III) and ytterbium(III). <i>Chemical Physics Letters</i> , 2007, 441, 354-357.	2.6	18
62	Momentum-space properties of the neutral atoms from H through U. <i>Atomic Data and Nuclear Data Tables</i> , 1991, 48, 213-229.	2.4	17
63	Modeling lanthanide coordination compounds: Sparkle/AM1 parameters for praseodymium (III). <i>Journal of Organometallic Chemistry</i> , 2005, 690, 4099-4102.	1.8	17
64	Modeling rare earth complexes: Sparkle/AM1 parameters for thulium (III). <i>Chemical Physics Letters</i> , 2005, 411, 61-65.	2.6	17
65	Theoretical and experimental luminescence quantum yields of coordination compounds of trivalent europium. <i>International Journal of Quantum Chemistry</i> , 2005, 103, 572-579.	2.0	17
66	1,3-thiazolium-5-thiolates mesoionic compounds: semiempirical evaluation of their first static hyperpolarizabilities and synthesis of new examples. <i>Journal of the Brazilian Chemical Society</i> , 2010, 21, 934-940.	0.6	17
67	Momentum space properties of atoms. <i>International Journal of Quantum Chemistry</i> , 1983, 23, 811-820.	2.0	16
68	Probing the nuclear susceptibility of mesoionic compounds using two-beam coupling with chirp-controlled pulses. <i>Chemical Physics Letters</i> , 2007, 449, 101-106.	2.6	16
69	Partial-wave analysis of the momentum densities of 14 electron diatomics. <i>International Journal of Quantum Chemistry</i> , 1984, 26, 385-392.	2.0	15
70	Ultrafast dynamics of mesoionic liquid solutions studied with incoherent light. <i>Chemical Physics Letters</i> , 2001, 347, 163-166.	2.6	15
71	Synthesis, Characterization and Crystallographic Studies of Three 2-Aryl-3-methyl-4-aryl-1,3-thiazolium-5-thiolates. <i>Synthesis</i> , 2003, 2003, 0685-0690.	2.3	15
72	Sparkle/AM1 modeling of holmium (III) complexes. <i>Polyhedron</i> , 2005, 24, 3046-3051.	2.2	15

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73	Sparkle model for the AM1 calculation of dysprosium (III) complexes. Inorganic Chemistry Communication, 2005, 8, 831-835.	3.9	15
74	Many-body perturbation theory and coupled-cluster calculations of the ground-state structure of CO <sub>3</sub> . Chemical Physics Letters, 1991, 177, 98-102.	2.6	14
75	Mesoionic Compounds: Amphiphilic Heterocyclic Betaines. Synthesis, 2000, 2000, 1565-1568.	2.3	13
76	Cerium (III) Complexes Modeling with Sparkle/PM3. Lecture Notes in Computer Science, 2007, , 312-318.	1.3	13
77	Substituent effects in alkynes and cyanides: a momentum density perspective. Canadian Journal of Chemistry, 1985, 63, 1412-1417.	1.1	12
78	The quality of s-orbitals determined by least-squares fitting and constrained variational methods. International Journal of Quantum Chemistry, 1986, 30, 717-735.	2.0	12
79	Uma metodologia para o projeto teórico de conversores moleculares de luz. Quimica Nova, 1998, 21, 51-59.	0.3	12
80	Reverse saturable absorption and anti-Stokes fluorescence in mesoionic compounds pumped at 532 nm. Applied Optics, 2001, 40, 1389.	2.1	12
81	The lanthanide contraction within the sparkle model. International Journal of Quantum Chemistry, 2011, 111, 1734-1739.	2.0	12
82	Diffusion, reaction kinetics and exchange of sodium in aqueous solutions containing a crown ether. Chemical Physics Letters, 2001, 335, 43-49.	2.6	11
83	Theoretical nonlinear optics equivalence between mesoionic and polyenic bridges in push-pull compounds. Journal of the Brazilian Chemical Society, 2005, 16, 583-588.	0.6	11
84	Synthesis of mixed ligand europium complexes: Verification of predicted luminescence intensification. Journal of Luminescence, 2016, 170, 505-512.	3.1	11
85	The nodal structure of the momentum distributions of molecules. International Journal of Quantum Chemistry, 1984, 25, 1035-1044.	2.0	10
86	Electron-nuclear cusp check for self-consistent field wave functions for the neutral atoms from helium to uranium. Canadian Journal of Physics, 1986, 64, 1351-1352.	1.1	10
87	Generator coordinate gaussian expanded natural orbitals. Computational and Theoretical Chemistry, 1990, 210, 63-70.	1.5	10
88	Self-diffusion of Alkali Ions in Aqueous Solutions of Crown Ether Complexes. Journal of Physical Chemistry A, 2002, 106, 589-594.	2.5	10
89	Semiempirical Quantum Chemistry Model for the Lanthanides: RM1 (Recife Model 1) Parameters for Dysprosium, Holmium and Erbium. PLoS ONE, 2014, 9, e86376.	2.5	10
90	Faster Synthesis of Beta-Diketonate Ternary Europium Complexes: Elapsed Times & Reaction Yields. PLoS ONE, 2015, 10, e0143998.	2.5	10

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91	Relativistic integrals over Breit-Pauli operators. <i>Journal of Chemical Physics</i> , 1984, 81, 5219-5221.	3.0	8
92	Substantial luminescence enhancement in ternary europium complexes by coordination of different ionic ligands. <i>RSC Advances</i> , 2016, 6, 90934-90943.	3.6	8
93	Stereoisomerism in Lanthanide Complexes: Enumeration, Chirality, Identification, Random Coordination Ratios. <i>Inorganic Chemistry</i> , 2018, 57, 10557-10567.	4.0	8
94	Synthesis and complete assignments of <sup>1</sup> H and <sup>13</sup> C NMR spectra of mesoionic 1,3-thiazolium-2 thiolates. <i>Arkivoc</i> , 2004, 2004, 12-21.	0.5	7
95	Infrared intensity parameters for furan and thiophene. <i>Computational and Theoretical Chemistry</i> , 1991, 235, 185-188.	1.5	6
96	SYNTHESIS AND CHARACTERIZATION OF MESOIONIC 1,3,4-TRIAZOLIUM-2-SELENOLATES. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2000, 161, 115-121.	1.6	6
97	Two-Photon Absorption Cross-Sections from Electronic Structure Methods: Mesoionic Compounds. <i>Chemistry of Materials</i> , 2008, 20, 4142-4155.	6.7	6
98	Europium complexes: choice of efficient synthetic routes from RM1 thermodynamic quantities as figures of merit. <i>RSC Advances</i> , 2017, 7, 20811-20823.	3.6	6
99	RM1 Semiempirical Model: Chemistry, Pharmaceutical Research, Molecular Biology and Materials Science. <i>Journal of the Brazilian Chemical Society</i> , 2018, , .	0.6	6
100	A momentum density analysis of strong hydrogen bonding. <i>Computational and Theoretical Chemistry</i> , 1985, 123, 221-229.	1.5	5
101	B3LYP, RHF and PM5 theoretical studies on phosphorescent cyclometalated Ir(III) complexes. <i>Chemical Physics Letters</i> , 2006, 420, 230-234.	2.6	5
102	RM1 Semiempirical Quantum Chemistry: Parameters for Trivalent Lanthanum, Cerium and Praseodymium. <i>PLoS ONE</i> , 2015, 10, e0124372.	2.5	5
103	A theorized new class of polyhedral hydrocarbons of molecular formula C <sub>n</sub> H <sub>n</sub> and their bottom-up scaffold expansions into hyperstructures. <i>Scientific Reports</i> , 2021, 11, 5576.	3.3	5
104	Molecular modeling of the octacoordinated tetracarbonato-Nd(III), [Nd(CO <sub>3</sub> ) <sub>4</sub> ] <sup>5-</sup> , complex and its nonacoordinated fluoro- and aquo-adducts. <i>Journal of Rare Earths</i> , 2010, 28, 847-853.	4.8	3
105	NMR and luminescence experiments reveal the structure and symmetry adaptation of a europium ionic liquid to solvent polarity. <i>Dalton Transactions</i> , 2021, 50, 10193-10205.	3.3	3
106	Parameters for the RM1 Quantum Chemical Calculation of Complexes of the Trications of Thulium, Ytterbium and Lutetium. <i>PLoS ONE</i> , 2016, 11, e0154500.	2.5	3
107	RM1 modeling of neodymium, promethium, and samarium coordination compounds. <i>RSC Advances</i> , 2015, 5, 12403-12408.	3.6	2
108	The complex build algorithm to set up starting structures of lanthanoid complexes with stereochemical control for molecular modeling. <i>Scientific Reports</i> , 2021, 11, 21493.	3.3	2

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109	A Gaussian quadrature for the optimal evaluation of integrals involving Lorentzians over a semi-infinite interval. <i>Computer Physics Communications</i> , 1991, 62, 16-24.	7.5	1
110	Validity of the mass-velocity term in the Breit-Pauli hamiltonian. <i>International Journal of Quantum Chemistry</i> , 1985, 28, 61-68.	2.0	1
111	Appraisal of computer hardware and software for quantum-chemical calculations. <i>International Journal of Quantum Chemistry</i> , 1984, 26, 619-638.	2.0	0
112	Comparison between the theoretical models and experimental structures of some octacoordinated Ln(III)-bis-dipyridyl-bis-dichloroacetato-diaquo complexes and their phenanthroline analogues. <i>Journal of Rare Earths</i> , 2010, 28, 83-85.	4.8	0
113	Quantum molecular mechanics—a noniterative procedure for the fast <i>Ab Initio</i> calculation of closed shell systems. <i>Journal of Computational Chemistry</i> , 2012, 33, 958-969.	3.3	0
114	Effects of crystal lattice and counterions on the geometries of metal complexes: Hexaaquamagnesium cation as a case study. <i>Journal of Molecular Structure</i> , 2017, 1134, 458-463.	3.6	0