Gerd B Rocha

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/2301374/publications.pdf

Version: 2024-02-01

70	2,465	304368	205818
papers	citations	22 h-index	48 g-index

70	70	70	2679
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Discovery of RTA ricin subunit inhibitors: a computational study using PM7 quantum chemical method and steered molecular dynamics. Journal of Biomolecular Structure and Dynamics, 2022, 40, 5427-5445.	2.0	4
2	A higher flexibility at the SARS-CoV-2 main protease active site compared to SARS-CoV and its potentialities for new inhibitor virtual screening targeting multi-conformers. Journal of Biomolecular Structure and Dynamics, 2022, 40, 9214-9234.	2.0	7
3	Investigation of the structural dynamics of a knotted protein and its unknotted analog using molecular dynamics. Journal of Molecular Modeling, 2022, 28, 108.	0.8	0
4	Thermochemical and Quantum Descriptor Calculations for Gaining Insight into Ricin Toxin A (RTA) Inhibitors. ACS Omega, 2021, 6, 8764-8777.	1.6	6
5	Synthesis, spectroscopic characterization, DFT calculations, and molecular docking studies of new unsymmetric bishydrazone derivatives. Journal of Molecular Structure, 2021, 1244, 131224.	1.8	13
6	Repurposing approved drugs as inhibitors of SARS-CoV-2â€‰S-protein from molecular modeling and virtual screening. Journal of Biomolecular Structure and Dynamics, 2021, 39, 3924-3933.	2.0	102
7	Elucidating Enzymatic Catalysis Using Fast Quantum Chemical Descriptors. Journal of Chemical Information and Modeling, 2020, 60, 578-591.	2.5	17
8	Theoretical characterization of the shikimate 5-dehydrogenase reaction from Mycobacterium tuberculosis by hybrid QC/MM simulations and quantum chemical descriptors. Journal of Molecular Modeling, 2020, 26, 297.	0.8	7
9	PRIMoRDiA: A Software to Explore Reactivity and Electronic Structure in Large Biomolecules. Journal of Chemical Information and Modeling, 2020, 60, 5885-5890.	2.5	6
10	GPU algorithms for density matrix methods on MOPAC: linear scaling electronic structure calculations for large molecular systems. Journal of Molecular Modeling, 2020, 26, 313.	0.8	6
11	Semiempirical methods do Fukui functions: Unlocking a modeling framework for biosystems. Journal of Computational Chemistry, 2020, 41, 862-873.	1.5	12
12	Synthesis, spectroscopic characterization, DFT studies, and preliminary antimicrobial evaluation of new antimony(III) and bismuth(III) complexes derived from 1,3,5-triazine. Journal of Molecular Structure, 2019, 1183, 373-383.	1.8	6
13	Synthesis, thermochemical and quantum chemical studies on antimony(III) and bismuth(III) complexes with 2,2â€²-bipyridine and 1,10-phenanthroline. Thermochimica Acta, 2019, 676, 234-240.	1.2	4
14	NAMD goes quantum: an integrative suite for hybrid simulations. Nature Methods, 2018, 15, 351-354.	9.0	149
15	RM1 Semiempirical Model: Chemistry, Pharmaceutical Research, Molecular Biology and Materials Science. Journal of the Brazilian Chemical Society, 2018, , .	0.6	6
16	Efficient algorithm for expanding theoretical electron densities in canterakisâ€“zernike functions. Journal of Computational Chemistry, 2018, 39, 2022-2032.	1.5	2
17	Determining the Relative Binding Affinity of Ricin Toxin A Inhibitors by Using Molecular Docking and Nonequilibrium Work. Journal of Chemical Information and Modeling, 2018, 58, 1205-1213.	2.5	10
18	Spin states of Mn(III) meso-tetraphenylporphyrin chloride assessed by density functional methods. Journal of Molecular Modeling, 2017, 23, 363.	0.8	2

#	Article	IF	Citations
19	Assessment of semiempirical enthalpy of formation in solution as an effective energy function to discriminate nativeâ€like structures in protein decoy sets. Journal of Computational Chemistry, 2016, 37, 1962-1972.	1.5	9
20	Parameters for the RM1 Quantum Chemical Calculation of Complexes of the Trications of Thulium, Ytterbium and Lutetium. PLoS ONE, 2016, 11, e0154500.	1.1	3
21	RM1 Semiempirical Quantum Chemistry: Parameters for Trivalent Lanthanum, Cerium and Praseodymium. PLoS ONE, 2015, 10, e0124372.	1.1	5
22	A topological assessment of the electronic structure of mesoionic compounds. Journal of Computational Chemistry, 2015, 36, 1907-1918.	1.5	4
23	RM1 modeling of neodymium, promethium, and samarium coordination compounds. RSC Advances, 2015, 5, 12403-12408.	1.7	2
24	Semiempirical Quantum Chemistry Model for the Lanthanides: RM1 (Recife Model 1) Parameters for Dysprosium, Holmium and Erbium. PLoS ONE, 2014, 9, e86376.	1.1	10
25	RM1 Model for the Prediction of Geometries of Complexes of the Trications of Eu, Gd, and Tb. Journal of Chemical Theory and Computation, 2014, 10, 3031-3037.	2.3	36
26	Sparkle/RM1 parameters for the semiempirical quantum chemical calculation of lanthanide complexes. RSC Advances, 2013, 3, 16747.	1.7	58
27	Performance assessment of semiempirical molecular orbital methods in the structural prediction of Sb(III) and Bi(III) complexes. Journal of Molecular Modeling, 2013, 19, 4575-4584.	0.8	2
28	Sparkle/PM7 Lanthanide Parameters for the Modeling of Complexes and Materials. Journal of Chemical Theory and Computation, 2013, 9, 3333-3341.	2.3	107
29	Sparse Projected-Gradient Method As a Linear-Scaling Low-Memory Alternative to Diagonalization in Self-Consistent Field Electronic Structure Calculations. Journal of Chemical Theory and Computation, 2013, 9, 1043-1051.	2.3	11
30	GPU Linear Algebra Libraries and GPGPU Programming for Accelerating MOPAC Semiempirical Quantum Chemistry Calculations. Journal of Chemical Theory and Computation, 2012, 8, 3072-3081.	2.3	222
31	DFT/PCM, QTAIM, 1H NMR conformational studies and QSAR modeling of thirty-two anti-Leishmania amazonensis Moritaâ€“Baylisâ€“Hillman Adducts. Journal of Molecular Structure, 2012, 1022, 72-80.	1.8	11
32	A DFT and Natural Resonance Theory investigation of the electronic structure of mesoionic compounds. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	12
33	Would the solvent effect be the main cause of band shift in the theoretical absorption spectrum of large lanthanide complexes?. Journal of Molecular Structure, 2011, 997, 30-36.	1.8	4
34	3-Hydroxy-2-methylene-3-(4-nitrophenylpropanenitrile): A new highly active compound against epimastigote and trypomastigote form of Trypanosoma cruzi. Bioorganic Chemistry, 2010, 38, 190-195.	2.0	21
35	Efficient synthesis of 16 aromatic Moritaâ€“Baylisâ€“Hillman adducts: Biological evaluation on Leishmania amazonensis and Leishmania chagasi. Bioorganic Chemistry, 2010, 38, 279-284.	2.0	25
36	1,3-thiazolium-5-thiolates mesoionic compounds: semiempirical evaluation of their first static hyperpolarizabilities and synthesis of new examples. Journal of the Brazilian Chemical Society, 2010, 21, 934-940.	0.6	17

#	Article	IF	Citations
37	Revisiting the origin of the preferential Ï€-Ï€ stacking conformation of the (+)-8-phenylmenthyl acrylate. Journal of the Brazilian Chemical Society, 2010, 21, 1718-1726.	0.6	19
38	Sparkle/PM3 for the modeling of europium(III), gadolinium(III), and terbium(III) complexes. Journal of the Brazilian Chemical Society, 2009, 20, 1638-1645.	0.6	59
39	Lanthanide coordination compounds modeling: Sparkle/PM3 parameters for dysprosium (III), holmium (III) and erbium (III). Journal of Organometallic Chemistry, 2008, 693, 1952-1956.	0.8	22
40	Sparkle/PM3 Parameters for the Modeling of Neodymium(III), Promethium(III), and Samarium(III) Complexes. Journal of Chemical Theory and Computation, 2007, 3, 1588-1596.	2.3	27
41	Structure Modeling of Trivalent Lanthanum and Lutetium Complexes:â€‰ Sparkle/PM3. Journal of Physical Chemistry A, 2007, 111, 5015-5018.	1.1	23
42	Sparkle/PM3 parameters for praseodymium(III) and ytterbium(III). Chemical Physics Letters, 2007, 441, 354-357.	1.2	18
43	Synthesis and conformational study of a new class of highly bioactive compounds. Chemical Physics Letters, 2007, 449, 336-340.	1.2	31
44	Cerium (III) Complexes Modeling with Sparkle/PM3. Lecture Notes in Computer Science, 2007, , 312-318.	1.0	13
45	Sparkle/AM1 Structure Modeling of Lanthanum (III) and Lutetium (III) Complexes. Journal of Physical Chemistry A, 2006, 110, 5897-5900.	1.1	28
46	Sparkle/AM1 Parameters for the Modeling of Samarium(III) and Promethium(III) Complexes. Journal of Chemical Theory and Computation, 2006, 2, 64-74.	2.3	37
47	B3LYP, RHF and PM5 theoretical studies on phosphorescent cyclometalated Ir(III) complexes. Chemical Physics Letters, 2006, 420, 230-234.	1.2	5
48	Modeling rare earth complexes: Sparkle/PM3 parameters for thulium(III). Chemical Physics Letters, 2006, 425, 138-141.	1.2	36
49	AM1 Sparkle modeling of Er(III) and Ce(III) coordination compounds. Journal of Organometallic Chemistry, 2006, 691, 2584-2588.	0.8	22
50	Sparkle model for AM1 calculation of neodymium(III) coordination compounds. Journal of Photochemistry and Photobiology A: Chemistry, 2006, 177, 225-237.	2.0	23
51	Lanthanide complex coordination polyhedron geometry prediction accuracies of ab initio effective core potential calculations. Journal of Molecular Modeling, 2006, 12, 373-389.	0.8	56
52	RM1: A reparameterization of AM1 for H, C, N, O, P, S, F, Cl, Br, and I. Journal of Computational Chemistry, 2006, 27, 1101-1111.	1.5	634
53	Modeling lanthanide coordination compounds: Sparkle/AM1 parameters for praseodymium (III). Journal of Organometallic Chemistry, 2005, 690, 4099-4102.	0.8	17
54	Efficacy of the semiempirical sparkle model as compared to ECP ab-initio calculations for the prediction of ligand field parameters of europium (III) complexes. Journal of Luminescence, 2005, 111, 81-87.	1.5	32

#	Article	IF	Citations
55	Synthesis, characterization and spectroscopic study of Eu(III) complexes with 3-aminopicolinic acid derivatives. Journal of Luminescence, 2005, 113, 79-88.	1.5	3
56	Sparkle/AM1 modeling of holmium (III) complexes. Polyhedron, 2005, 24, 3046-3051.	1.0	15
57	Sparkle model for the AM1 calculation of dysprosium (III) complexes. Inorganic Chemistry Communication, 2005, 8, 831-835.	1.8	15
58	On the use of combinatory chemistry to the design of new luminescent Eu3+ complexes. Chemical Physics Letters, 2005, 405, 123-126.	1.2	35
59	Modeling rare earth complexes: Sparkle/AM1 parameters for thulium (III). Chemical Physics Letters, 2005, 411, 61-65.	1.2	17
60	Modeling lanthanide complexes: Sparkle/AM1 parameters for ytterbium (III). Journal of Computational Chemistry, 2005, 26, 1524-1528.	1.5	18
61	Synthesis and Luminescent Properties of Novel Europium(III) Heterocyclic Î²-Diketone Complexes with Lewis Bases: Structural Analysis Using the Sparkle/AM1 Model. European Journal of Inorganic Chemistry, 2005, 2005, 4129-4137.	1.0	47
62	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
63	Sparkle Model for the Calculation of Lanthanide Complexes:Â AM1 Parameters for Eu(III), Gd(III), and Tb(III)â€. Inorganic Chemistry, 2005, 44, 3299-3310.	1.9	133
64	Sparkle Model for AM1 Calculation of Lanthanide Complexes:Â Improved Parameters for Europiumâ€. Inorganic Chemistry, 2004, 43, 2346-2354.	1.9	65
65	Reverse saturable absorption and anti-Stokes fluorescence in mesoionic compounds pumped at 532 nm. Applied Optics, 2001, 40, 1389.	2.1	12
66	On the charge factors of the simple overlap model for the ligand field in lanthanide coordination compounds. Chemical Physics Letters, 2000, 331, 519-525.	1.2	43
67	Design of ligands to obtain lanthanide ion complexes displaying high quantum efficiencies of luminescence using the sparkle model. Computational and Theoretical Chemistry, 2000, 527, 245-251.	1.5	30
68	Synthesis, Spectroscopic Characterization, DFT Calculations and Preliminary Antifungal Activity of New Piperine Derivatives. Journal of the Brazilian Chemical Society, 0, , .	0.6	0
69	Synthesis, in silico Study, Theoretical Stereochemistry Elucidation and Antifungal Activity of New Imides Derived from Safrole. Journal of the Brazilian Chemical Society, 0, , .	0.6	1
70	A Simple Strategy That Uses Molecular Dynamics and Semiempirical Methods for the Conformational Searching of isomers of the Macrocycle Complex Na[Gd(DOTA)Â·H2O]. Revista Virtual De Quimica, 0, , 641-655.	0.1	0