Luis Rodriguez-Santiago

List of Publications by Year
in descending order

75 papers	2,867 citations	147801 31 h-index	182427 51 g-index
78 all docs	78 docs citations	78 times ranked	2618 citing authors

#	Article	IF	Citations
1	Ground State of the (H2O)2+ Radical Cation:â€‰ DFT versus Post-Hartreeâ€“Fock Methods. Journal of Physical Chemistry A, 1999, 103, 166-170.	2.5	232
2	Single versus Double Proton-Transfer Reactions in Watsonâ€“Crick Base Pair Radical Cations. A Theoretical Study. Journal of the American Chemical Society, 1998, 120, 8159-8167.	13.7	203
3	The Different Nature of Bonding in Cu+-Glycine and Cu2+-Glycine. Journal of Physical Chemistry B, 1999, 103, 2310-2317.	2.6	198
4	Coordination of Cu+Ions to Zeolite Frameworks Strongly Enhances Their Ability To Bind NO2. An ab Initio Density Functional Study. Journal of the American Chemical Society, 1998, 120, 1545-1551.	13.7	109
5	Ground and Low-Lying States of Cu2+â€“H2O. A Difficult Case for Density Functional Methods. Journal of Physical Chemistry A, 2004, 108, 6072-6078.	2.5	85
6	Differences in the Activation Processes of Phosphine-Containing and Grubbsâ€“Hoveyda-Type Alkene Metathesis Catalysts. Organometallics, 2012, 31, 4203-4215.	2.3	85
7	Protonation of glycine, serine and cysteine. Conformations, proton affinities and intrinsic basicities. Computational and Theoretical Chemistry, 2001, 537, 307-318.	1.5	83
8	Crystal structure of thioflavin-T and its binding to amyloid fibrils: insights at the molecular level. Chemical Communications, 2010, 46, 1156.	4.1	78
9	Cationâ€“Ï€ Interactions and Oxidative Effects on Cu+and Cu2+Binding to Phe, Tyr, Trp, and His Amino Acids in the Gas Phase. Insights from First-Principles Calculations. Journal of Physical Chemistry B, 2006, 110, 24189-24199.	2.6	77
10	Gas-Phase Reactivity of Ni+with Glycine. Journal of Physical Chemistry A, 2001, 105, 5340-5347.	2.5	66
11	Three Dimensional Models of Cu²⁺-Aî²(1â€“16) Complexes from Computational Approaches. Journal of the American Chemical Society, 2011, 133, 15008-15014.	13.7	61
12	Gas Phase Intramolecular Proton Transfer in Cationized Glycine and Chlorine Substituted Derivatives (Mâ€“Gly, M=Na+, Mg2+, Cu+, Ni+, and Cu2+): Existence of Zwitterionic Structures?. Chemistry - A European Journal, 2000, 6, 4393-4399.	3.3	60
13	Intramolecular Proton Transfer in Glycine Radical Cation. Journal of Physical Chemistry A, 2000, 104, 1256-1261.	2.5	59
14	Mechanistic Insights into Ringâ€Closing Enyne Metathesis with the Secondâ€Generation Grubbsâ€“Hoveyda Catalyst: A DFT Study. Chemistry - A European Journal, 2011, 17, 7506-7520.	3.3	56
15	Thioflavin-T excimer formation upon interaction with amyloid fibers. Chemical Communications, 2013, 49, 5745.	4.1	56
16	Computational calculations of pKa values of imidazole in Cu(ii) complexes of biological relevance. Physical Chemistry Chemical Physics, 2011, 13, 7852.	2.8	55
17	Solvent-assisted catalysis in the enolization of acetaldehyde radical cation. Chemical Physics Letters, 2001, 334, 112-118.	2.6	52
18	pH-Responsive Self-Assembly of Amyloid Fibrils for Dual Hydrolase-Oxidase Reactions. ACS Catalysis, 2021, 11, 595-607.	11.2	49

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19	Hydrogen Atom or Proton Transfer in Neutral and Single Positive Ions of Salicylic Acid and Related Compounds. Journal of the American Chemical Society, 1999, 121, 8882-8890.	13.7	48
20	Comparison of density functional and coupled cluster methods in the study of metalâ€“ligand systems: Scâ€“CO2 and Cuâ€“NO2. Journal of Chemical Physics, 1996, 105, 9966-9971.	3.0	46
21	Coordination Properties of the Oxime Analogue of Glycine to Cu(II). Journal of Physical Chemistry A, 2005, 109, 5668-5676.	2.5	46
22	The Role of Exact Exchange in the Description of Cu²⁺â^'(H₂O)_n(n= 1â^'6) Complexes by Means of DFT Methods. Journal of Physical Chemistry A, 2010, 114, 10857-10863.	2.5	43
23	Interaction of Co+ and Co2+ with Glycine. A Theoretical Study. Journal of Physical Chemistry A, 2005, 109, 224-230.	2.5	42
24	Influence of N7 Protonation on the Mechanism of the N-Glycosidic Bond Hydrolysis in 2â€˜-Deoxyguanosine. A Theoretical Study. Journal of Physical Chemistry B, 2007, 111, 6071-6077.	2.6	42
25	Influence of the Side Chain in the Structure and Fragmentation of Amino Acids Radical Cations. Journal of Chemical Theory and Computation, 2007, 3, 2210-2220.	5.3	41
26	On the Bonding of First-Row Transition Metal Cations to Guanine and Adenine Nucleobases. Journal of Physical Chemistry A, 2007, 111, 9823-9829.	2.5	34
27	Metal-Mediated Deamination of Cytosine: Experiment and DFT Calculations. Angewandte Chemie - International Edition, 2004, 43, 5396-5399.	13.8	33
28	Coordination properties of glycylglycine to Cu+, Ni+ and Co+. Influence of metal cation electronic configuration. New Journal of Chemistry, 2005, 29, 1585.	2.8	32
29	Is the Peptide Bond Formation Activated by Cu2+Interactions? Insights from Density Functional Calculations. Journal of Physical Chemistry B, 2007, 111, 5740-5747.	2.6	32
30	Toward Olefin Metathesis with Iron Carbene Complexes: Benefits of Tridentate Ïƒ-Donating Ligands. Organometallics, 2016, 35, 3914-3923.	2.3	32
31	Exo/endo Selectivity of the Ring-Closing Enyne Methathesis Catalyzed by Second Generation Ru-Based Catalysts. Influence of Reactant Substituents. ACS Catalysis, 2013, 3, 206-218.	11.2	31
32	DFT Study on the Relative Stabilities of Substituted Ruthenacyclobutane Intermediates Involved in Olefin Cross-Metathesis Reactions and Their Interconversion Pathways. Organometallics, 2014, 33, 6065-6075.	2.3	31
33	DFT Study on the Recovery of Hoveydaâ€“Grubbsâ€Type Catalyst Precursors in Enyne and Diene Ringâ€Closing Metathesis. Chemistry - A European Journal, 2013, 19, 14553-14565.	3.3	30
34	3D Structures and Redox Potentials of Cu²⁺â€“AÎ²(1â€“16) Complexes at Different pH: A Computational Study. Journal of Physical Chemistry B, 2014, 118, 4840-4850.	2.6	30
35	Water Adsorption on MO₂ (M = Ti, Ru, and Ir) Surfaces. Importance of Octahedral Distortion and Cooperative Effects. ACS Omega, 2019, 4, 2989-2999.	3.5	28
36	Structures and Stabilities of Fe2+/3+Complexes Relevant to Alzheimerâ€™s Disease: An ab Initio Study. Journal of Physical Chemistry A, 2011, 115, 12523-12530.	2.5	27

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37	Reactivity of Metal Carbenes with Olefins: Theoretical Insights on the Carbene Electronic Structure and Cyclopropanation Reaction Mechanism. Journal of Physical Chemistry A, 2018, 122, 1702-1712.	2.5	26
38	Effects of Ionization, Metal Cationization and Protonation on 2â€˜-Deoxyguanosine:Â Changes on Sugar Puckering and Stability of the N-Glycosidic Bond. Journal of Physical Chemistry B, 2006, 110, 5767-5772.	2.6	24
39	Gas phase reactivity of Cu+-aromatic amino acids. International Journal of Mass Spectrometry, 2006, 257, 60-69.	1.5	24
40	Dioxygen activation in the Cuâ€“amyloid Î² complex. Physical Chemistry Chemical Physics, 2015, 17, 27270-27274.	2.8	24
41	Drastic Effect of the Peptide Sequence on the Copperâ€Binding Properties of Tripeptides and the Electrochemical Behaviour of Their Copper(II) Complexes. Chemistry - A European Journal, 2018, 24, 5153-5162.	3.3	24
42	Thioflavin-based molecular probes for application in Alzheimer's disease: from in silico to in vitro models. Metallomics, 2015, 7, 83-92.	2.4	23
43	Theoretical study of the bonding of NO2 to Cu and Ag. Journal of Chemical Physics, 1995, 103, 9738-9743.	3.0	21
44	On the electronic structure of second generation Hoveydaâ€“Grubbs alkene metathesis precursors. Computational and Theoretical Chemistry, 2012, 996, 57-67.	2.5	21
45	Elucidating the 3D structures of Al(<scp>iii</scp>)â€“Aβ2 complexes: a template free strategy based on the pre-organization hypothesis. Chemical Science, 2017, 8, 5041-5049.	7.4	21
46	Binding Properties of Cu^{+/2+}-(glycyl)_nglycine Complexes (n =) Tj ETQq0 0 0 rgBT /Overlock 10 T	2.5	19
47	Structure, Bonding, and Relative Stability of the Ground and Low-Lying Electronic States of CuO2. The Role of Exact Exchange. Journal of Physical Chemistry A, 2009, 113, 1308-1317.	2.5	19
48	Insights on the Binding of Thioflavin Derivative Markers to Amyloid-Like Fibril Models from Quantum Chemical Calculations. Journal of Physical Chemistry B, 2013, 117, 6674-6680.	2.6	19
49	Gas Phase Reactivity of Ni+ with Urea. Mass Spectrometry and Theoretical Studies. Journal of Physical Chemistry A, 2003, 107, 9865-9874.	2.5	18
50	Importance of the oxyl character on the IrO2 surface dependent catalytic activity for the oxygen evolution reaction. Journal of Catalysis, 2021, 396, 192-201.	6.2	18
51	[2 + 2] Photocycloaddition of 2(5H)-Furanone to Unsaturated Compounds. Insights from First Principles Calculations and Transient-Absorption Measurements. Journal of Organic Chemistry, 2010, 75, 4392-4401.	3.2	17
52	Modeling Cu2+-Aβ2 complexes from computational approaches. AIP Advances, 2015, 5, 092402.	1.3	17
53	On the mechanism of the N-glycosydic bond hydrolysis of 2â€²-deoxyguanosine: insights from first principles calculations. Theoretical Chemistry Accounts, 2011, 128, 619-626.	1.4	14
54	Pt^{II} Coordination to N1 of 9â€Methylguanine: Why it Facilitates Binding of Additional Metal Ions to the Purine Ring. Chemistry - A European Journal, 2011, 17, 9970-9983.	3.3	14

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55	Influence of Ligands and Oxidation State on the Reactivity of Pentacoordinated Iron Carbenes with Olefins: Metathesis versus Cyclopropanation. Organometallics, 2018, 37, 1229-1241.	2.3	14
56	Coordination properties of a metal chelator clioquinol to Zn²⁺ studied by static DFT and ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2015, 17, 13582-13589.	2.8	13
57	BCN-M: A Free Computational Tool for Generating Wulff-like Nanoparticle Models with Controlled Stoichiometry. Journal of Physical Chemistry C, 2020, 124, 1227-1237.	3.1	13
58	Metal coordination determines the catalytic activity of IrO2 nanoparticles for the oxygen evolution reaction. Journal of Catalysis, 2022, 412, 78-86.	6.2	13
59	Coordination of NO2to Cu and Mg in M(NO2)2Complexes. A Theoretical Study. Inorganic Chemistry, 1998, 37, 4512-4517.	4.0	11
60	Influence of Ï€-stacking on the N7 and O6 proton affinity of guanine. Theoretical Chemistry Accounts, 2009, 123, 105-111.	1.4	11
61	Enhanced Metallophilicity in Metalâ€“Carbene Systems: Stronger Character of Aurophilic Interactions in Solution. Chemistry - A European Journal, 2020, 26, 997-1002.	3.3	11
62	Coordination of NO2to Alkaline-Earth Metals. A Theoretical Study. Journal of Physical Chemistry A, 1998, 102, 630-635.	2.5	10
63	Gas-Phase Reactivity of Cu+and Ag+with Glycerol:Â an Experimental and Theoretical Study. Journal of Physical Chemistry A, 2002, 106, 10563-10577.	2.5	9
64	Experimental and theoretical studies on the gas phase reactivity of formamideâ€“Ni+ complexes generated by FAB and electrospray ionization. International Journal of Mass Spectrometry, 2002, 219, 429-443.	1.5	9
65	Coordination Properties of Lysine Interacting with Co(I) and Co(II). A Theoretical and Mass Spectrometry Study. Journal of Physical Chemistry A, 2008, 112, 12385-12392.	2.5	9
66	Coordination of (Glycyl)_nglycine (n= 1â^'3) to Co⁺and Co²⁺. Journal of Physical Chemistry A, 2009, 113, 8883-8892.	2.5	9
67	Mixed Adenine/Guanine Quartets with Three transâ€‹a₂Pt^{II} (a=NH₃ or MeNH₂) Crossâ€‹Links: Linkage and Rotational Isomerism, Base Pairing, and Loss of NH₃. Chemistry - A European Journal, 2014, 20, 3394-3407.	3.3	9
68	Atomistic fibrillar architectures of polar prion-inspired heptapeptides. Chemical Science, 2020, 11, 13143-13151.	7.4	9
69	Stability of transient Cu+AÎ² (1â€“16) species and influence of coordination and peptide configuration on superoxide formation. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	8
70	Surface morphology controls water dissociation on hydrated IrO₂ nanoparticles. Nanoscale, 2021, 13, 14480-14489.	5.6	8
71	Multiple Condensation Reactions Involving Pt^{II}/Pd^{II}â^'OH₂, Ptâ^'NH₃, and Cytosineâ^'NH₂ Groups: New Twists in Cisplatinâ^'Nucleobase Chemistry. Chemistry - A European Journal, 2016, 22, 13653-13668.	3.3	7
72	The electronic spectra of CaN+2 and Ca(N2)+2. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1999, 55, 457-466.	3.9	5

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73	Intramolecular Photocycloaddition of 2(5H)-Furanones to Temporarily Tethered Terminal Alkenes as a Stereoselective Source of Enantiomerically Pure Polyfunctionalyzed Cyclobutanes. Journal of Organic Chemistry, 2018, 83, 3188-3199.	3.2	2
74	Computational simulations of copper complexes relevant to Alzheimer's disease. , 2014, , .		0
75	Frontispiece: Enhanced Metallophilicity in Metalâ€“Carbene Systems: Stronger Character of Aurophilic Interactions in Solution. Chemistry - A European Journal, 2020, 26, .	3.3	0