Ricardo A Mata

List of Publications by Year
in descending order

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99 papers	3,268 citations	147801 31 h-index	175258 52 g-index
107 all docs	107 docs citations	107 times ranked	3998 citing authors

#	Article	IF	Citations
1	Widespread occurrence of covalent lysineâ€“cysteine redox switches in proteins. Nature Chemical Biology, 2022, 18, 368-375.	8.0	34
2	Anomeric Stereoauxiliary Cleavage of the Câ^'N Bond of <scp>d</scp>â€Glucosamine for the Preparation of Imidazo[1,5â€a]pyridines. Chemistry - A European Journal, 2022, 28, .	3.3	10
3	Setting up the HyDRA blind challenge for the microhydration of organic molecules. Physical Chemistry Chemical Physics, 2022, 24, 11442-11454.	2.8	9
4	Ground-state destabilization by electrostatic repulsion is not a driving force in orotidine-5â€²-monophosphate decarboxylase catalysis. Nature Catalysis, 2022, 5, 332-341.	34.4	12
5	Ligand Protonation Triggers H₂ Release from a Dinickel Dihydride Complex to Give a Doubly â€œTâ€â€Shaped Dinickel(I) Metallodiradical. Angewandte Chemie - International Edition, 2021, 60, 1891-1896.	13.8	13
6	Time-Resolved Spectroscopy of Photoinduced Electron Transfer in Dinuclear and Tetranuclear Fe/Co Prussian Blue Analogues. Inorganic Chemistry, 2021, 60, 449-459.	4.0	18
7	Ligand Protonation Triggers H 2 Release from a Dinickel Dihydride Complex to Give a Doubly â€œTâ€â€Shaped Dinickel(I) Metallodiradical. Angewandte Chemie, 2021, 133, 1919-1924.	2.0	4
8	Dispersion forces in chirality recognition â€“ a density functional and wave function theory study of diols. Physical Chemistry Chemical Physics, 2021, 23, 12093-12104.	2.8	8
9	Theoretical Studies of the Acidâ€“Base Equilibria in a Model Active Site of the Human 20S Proteasome. Journal of Chemical Information and Modeling, 2021, 61, 1942-1953.	5.4	4
10	A lysineâ€“cysteine redox switch with an NOS bridge regulates enzyme function. Nature, 2021, 593, 460-464.	27.8	74
11	Inâ€Fjord Substitution in Expanded Helicenes: Effects of the Insert on the Inversion Barrier and Helical Pitch. Chemistry - A European Journal, 2021, 27, 13358-13366.	3.3	12
12	A Review of Density Functional Models for the Description of Fe(II) Spin-Crossover Complexes. Molecules, 2020, 25, 5176.	3.8	8
13	The first microsolvation step for furans: New experiments and benchmarking strategies. Journal of Chemical Physics, 2020, 152, 164303.	3.0	28
14	Electrophilic Cyanative Alkenylation of Arenes. Organic Letters, 2020, 22, 4932-4937.	4.6	8
15	Critical Assessment of RAFT Equilibrium Constants: Theory Meets Experiment. Macromolecular Theory and Simulations, 2020, 29, 2000022.	1.4	4
16	Photochemical Properties of Re(CO)₃ Complexes with and without a Local Proton Source and Implications for CO₂ Reduction Catalysis. Organometallics, 2020, 39, 2405-2414.	2.3	8
17	A high-throughput computational approach to UV-Vis spectra in protein mutants. Physical Chemistry Chemical Physics, 2019, 21, 20678-20692.	2.8	4
18	Low-barrier hydrogen bonds in enzyme cooperativity. Nature, 2019, 573, 609-613.	27.8	68

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19	A full additive QM/MM scheme for the computation of molecular crystals with extension to many-body expansions. Journal of Chemical Physics, 2019, 150, 154118.	3.0	6
20	Strained hydrogen bonding in imidazole trimer: a combined infrared, Raman, and theory study. Physical Chemistry Chemical Physics, 2019, 21, 5989-5998.	2.8	9
21	Limits of Coupled-Cluster Calculations for Non-Heme Iron Complexes. Journal of Chemical Theory and Computation, 2019, 15, 922-937.	5.3	51
22	The furan microsolvation blind challenge for quantum chemical methods: First steps. Journal of Chemical Physics, 2018, 148, 014301.	3.0	44
23	QM/MM study of the reaction mechanism of sulfite oxidase. Scientific Reports, 2018, 8, 4684.	3.3	22
24	Experimental charge density study on FLPs and a FLP reaction product. Zeitschrift Fur Kristallographie - Crystalline Materials, 2018, 233, 723-731.	0.8	2
25	Hybrid Local Molecular Orbital: Molecular Orbital Calculations for Open Shell Systems. Journal of Chemical Theory and Computation, 2018, 14, 5192-5202.	5.3	6
26	The phenyl vinyl etherâ€“methanol complex: a model system for quantum chemistry benchmarking. Beilstein Journal of Organic Chemistry, 2018, 14, 1642-1654.	2.2	12
27	All That Binds Is Not Goldâ€”The Relative Weight of Aurophilic Interactions in Complex Formation. Journal of Physical Chemistry A, 2018, 122, 6918-6925.	2.5	26
28	High level potential energy surface and mechanism of Al(CH3)2OCH3-promoted lactone polymerization: initiation and propagation. Physical Chemistry Chemical Physics, 2017, 19, 8989-8999.	2.8	4
29	Benchmarking Quantum Chemical Methods: Are We Heading in the Right Direction?. Angewandte Chemie - International Edition, 2017, 56, 11011-11018.	13.8	119
30	Theoretical Studies of the Electronic Absorption Spectra of Thiamin Diphosphate in Pyruvate Decarboxylase. Biochemistry, 2017, 56, 1854-1864.	2.5	10
31	Manganese(I)â€Catalyzed Dispersionâ€Enabled Cå^'H/Cå^'C Activation. Chemistry - A European Journal, 2017, 23, 5443-5447.	3.3	98
32	Dinuclear Rhenium Complex with a Proton Responsive Ligand as a Redox Catalyst for the Electrochemical CO₂ Reduction. Inorganic Chemistry, 2017, 56, 4176-4185.	4.0	50
33	Influence of size, shape, heteroatom content and dispersive contributions on guest binding in a coordination cage. Chemical Communications, 2017, 53, 11933-11936.	4.1	27
34	Pairwise H₂/D₂ Exchange and H₂ Substitution at a Bimetallic Dinickel(II) Complex Featuring Two Terminal Hydrides. Journal of the American Chemical Society, 2017, 139, 16720-16731.	13.7	36
35	Temperatureâ€Dependent Dynamics of Pushâ€“Pull Rotor Systems Based on Acridinylidene Cyanoacetic Esters. European Journal of Organic Chemistry, 2017, 2017, 5141-5146.	2.4	6
36	Lipoxygenase 2 from Cyanothece sp. controls dioxygen insertion by steric shielding and substrate fixation. Scientific Reports, 2017, 7, 2069.	3.3	14

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37	Quantenchemische Methoden im Leistungsvergleich: Stimmt die Richtung noch?. Angewandte Chemie, 2017, 129, 11155-11163.	2.0	14
38	Visualizing dispersion interactions through the use of local orbital spaces. Journal of Computational Chemistry, 2017, 38, 15-23.	3.3	37
39	Efficient parallelization of perturbative Monte Carlo QM/MM simulations in heterogeneous platforms. International Journal of High Performance Computing Applications, 2017, 31, 499-516.	3.7	1
40	Optimization and benchmarking of a perturbative Metropolis Monte Carlo quantum mechanics/molecular mechanics program. Journal of Chemical Physics, 2017, 147, 244105.	3.0	2
41	Solution Structures of Hauser Base ⁱPr₂NMgCl and Turbo-Hauser Base ⁱPr₂NMgClÂ·LiCl in THF and the Influence of LiCl on the Schlenk-Equilibrium. Journal of the American Chemical Society, 2016, 138, 4796-4806.	13.7	65
42	Internal dynamics and guest binding of a sterically overcrowded host. Chemical Science, 2016, 7, 4676-4684.	7.4	54
43	The inhibition mechanism of human 20 S proteasomes enables next-generation inhibitor design. Science, 2016, 353, 594-598.	12.6	170
44	Highly selective and sensitive fluorescence detection of Zn²⁺and Cd²⁺ions by using an acridine sensor. Dalton Transactions, 2016, 45, 5689-5699.	3.3	24
45	A Computational Comparison of Oxygen Atom Transfer Catalyzed by Dimethyl SulfÂoxide Reductase with Mo and W. European Journal of Inorganic Chemistry, 2015, 2015, 3580-3589.	2.0	23
46	FJK - A cap-free fragment approach with embedding Fock potentials. AIP Conference Proceedings, 2015, , .	0.4	0
47	Soft hydrogen bonds to alkenes: the methanolâ€“ethene prototype under experimental and theoretical scrutiny. Chemical Science, 2015, 6, 3738-3745.	7.4	26
48	Bracketing subtle conformational energy differences between self-solvated and stretched trifluoropropanol. Physical Chemistry Chemical Physics, 2015, 17, 9899-9909.	2.8	8
49	Helium Nanodroplet Study of the Hydrogen-Bonded OH Vibrations in HClâ€“H₂O Clusters. Journal of Physical Chemistry A, 2015, 119, 2636-2643.	2.5	7
50	Functional Model for the [Fe] Hydrogenase Inspired by the Frustrated Lewis Pair Concept. Journal of the American Chemical Society, 2014, 136, 16626-16634.	13.7	63
51	Local Hybrid QM/QM Calculations of Reaction Pathways in Metallobiosites. Journal of Chemical Theory and Computation, 2014, 10, 5397-5404.	5.3	10
52	Communication: Towards the binding energy and vibrational red shift of the simplest organic hydrogen bond: Harmonic constraints for methanol dimer. Journal of Chemical Physics, 2014, 141, 101105.	3.0	28
53	Coupledâ€Cluster Interaction Energies for 200â€Atom Hostâ€“Guest Systems. ChemPhysChem, 2014, 15, 3270-3281.	2.1	18
54	Characterization of a Multicomponent Lithium Lithiate from a Combined Xâ€Ray Diffraction, NMR Spectroscopy, and Computational Approach. Angewandte Chemie - International Edition, 2014, 53, 13282-13287.	13.8	20

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55	A quantum-mechanical study of the reaction mechanism of sulfite oxidase. Journal of Biological Inorganic Chemistry, 2014, 19, 1165-1179.	2.6	23
56	Free-energy perturbation and quantum mechanical study of SAMPL4 octa-acid hostâ€“guest binding energies. Journal of Computer-Aided Molecular Design, 2014, 28, 375-400.	2.9	70
57	Effects of Metal Coordination on the Ï€-System of the 2,5-Bis-{(pyrrolidino)-methyl}-pyrrole Pincer Ligand. Inorganic Chemistry, 2013, 52, 9539-9548.	4.0	23
58	Strong Intermolecular Interactions Shaping a Small Pianoâ€Stool Complex. Angewandte Chemie - International Edition, 2013, 52, 10365-10369.	13.8	12
59	Relative anion binding affinity in a series of interpenetrated coordination cages. Dalton Transactions, 2013, 42, 15906.	3.3	31
60	Study of ligand effects in aurophilic interactions using local correlation methods. Physical Chemistry Chemical Physics, 2013, 15, 18115.	2.8	37
61	Heteroaromaticity approached by charge density investigations and electronic structure calculations. Physical Chemistry Chemical Physics, 2013, 15, 20600.	2.8	27
62	The Layered Structure of [Na(NH₃)₄][Indenide] Containing a Squareâ€Planar Na(NH₃)₄⁺ Cation. Angewandte Chemie - International Edition, 2013, 52, 734-738.	13.8	15
63	Reaction of Nâ€Heterocyclic Silylenes with Thioketone: Formation of Siliconâ€“Sulfur Three (Siâ€Câ€S)â€and Five (Siâ€Câ€Câ€Câ€S)â€Membered Ring Systems. Chemistry - A European Journal, 2013, 19, 3715-3720.	3.3	22
64	Large Density-Functional and Basis-Set Effects for the DMSO Reductase Catalyzed Oxo-Transfer Reaction. Journal of Chemical Theory and Computation, 2013, 9, 1799-1807.	5.3	42
65	The Last Globally Stable Extended Alkane. Angewandte Chemie - International Edition, 2013, 52, 463-466.	13.8	105
66	Accelerating the Computation of Induced Dipoles for Molecular Mechanics with Dataflow Engines. , 2013, , .		8
67	Preorganized Anion Traps for Exploiting Anionâ€“Ï€ Interactions: An Experimental and Computational Study. Chemistry - A European Journal, 2013, 19, 16988-17000.	3.3	27
68	Ein kleiner Klavierstuhlâ€Komplex, geformt durch starke intermolekulare Wechselwirkungen. Angewandte Chemie, 2013, 125, 10555-10559.	2.0	10
69	Monomeric Sn(ii) and Ge(ii) hydrides supported by a tridentate pincer-based ligand. Chemical Communications, 2012, 48, 4890.	4.1	53
70	A push-and-pull model for allosteric anion binding in cage complexes. Physical Chemistry Chemical Physics, 2012, 14, 12746.	2.8	22
71	Structural diversity in sodium doped water trimers. Physical Chemistry Chemical Physics, 2012, 14, 9054.	2.8	25
72	Study of Specific Ionâ€“Amino Acid Interactions through the Use of Local Correlation Methods. Journal of Physical Chemistry A, 2012, 116, 5464-5471.	2.5	4

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73	Application of Local Second-Order MÃ¸llerâ€“Plesset Perturbation Theory to the Study of Structures in Solution. Journal of Chemical Theory and Computation, 2012, 8, 3053-3060.	5.3	4
74	Atomdroid: A Computational Chemistry Tool for Mobile Platforms. Journal of Chemical Information and Modeling, 2012, 52, 1072-1078.	5.4	12
75	Computation of Induced Dipoles in Molecular Mechanics Simulations Using Graphics Processors. Journal of Chemical Information and Modeling, 2012, 52, 1159-1166.	5.4	3
76	Photoionization of CH₃N₃ Produces ³B₂ N₃^{â€“}: A Theoretical and Experimental Study of the Ion-Pair Channel. Journal of Physical Chemistry Letters, 2011, 2, 2311-2315.	4.6	8
77	Does DFT-D estimate accurate energies for the binding of ligands to metal complexes?. Dalton Transactions, 2011, 40, 11176.	3.3	81
78	Preparation of RSn(I)â€“Sn(I)R with Two Unsymmetrically Coordinated Sn(I) Atoms and Subsequent Gentle Activation of P₄. Journal of the American Chemical Society, 2011, 133, 17889-17894.	13.7	105
79	A Stable Cation of a CSi₃P Fiveâ€Membered Ring with a Weakly Coordinating Chloride Anion. Angewandte Chemie - International Edition, 2011, 50, 12510-12513.	13.8	35
80	Synthesis and Structural Characterization of Homochiral Homoâ€oligomers of Parent cisâ€•and transâ€Furanoidâ€Î²â€Amino Acids. Chemistry - A European Journal, 2011, 17, 12946-12954.	3.3	24
81	An incremental correlation approach to excited state energies based on natural transition/localized orbitals. Journal of Chemical Physics, 2011, 134, 034122.	3.0	47
82	Reductive half-reaction of aldehyde oxidoreductase toward acetaldehyde: Ab initio and free energy quantum mechanical/molecular mechanical calculations. Journal of Chemical Physics, 2010, 132, 035101.	3.0	33
83	Iterative induced dipoles computation for molecular mechanics on GPUs. , 2010, , .		5
84	QM/MM Approaches to the Electronic Spectra of Hydrogen-Bonding Systems with Connection to Many-Body Decomposition Schemes. Advances in Quantum Chemistry, 2010, , 99-144.	0.8	4
85	Application of high level wavefunction methods in quantum mechanics/molecular mechanics hybrid schemes. Physical Chemistry Chemical Physics, 2010, 12, 5041.	2.8	18
86	Assessing the accuracy of many-body expansions for the computation of solvatochromic shifts. Molecular Physics, 2010, 108, 381-392.	1.7	8
87	Dynamic polarizability, Cauchy moments, and the optical absorption spectrum of liquid water: A sequential molecular dynamics/quantum mechanical approach. Journal of Chemical Physics, 2009, 130, 014505.	3.0	24
88	A Simple One-Body Approach to the Calculation of the First Electronic Absorption Band of Water. Journal of Chemical Theory and Computation, 2009, 5, 1829-1837.	5.3	30
89	Electronic Excitation of Cl^{â˜’} in Liquid Water and at the Surface of a Cluster: A Sequential Bornâ˜’Oppenheimer Molecular Dynamics/Quantum Mechanics Approach. Journal of Physical Chemistry A, 2009, 113, 14684-14690.	2.5	15
90	Incremental expansions for SCF interaction energies: A comparison for hydrogen-bonded clusters. Chemical Physics Letters, 2008, 465, 136-141.	2.6	20

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91	Toward accurate barriers for enzymatic reactions: QM/MM case study on p-hydroxybenzoate hydroxylase. Journal of Chemical Physics, 2008, 128, 025104.	3.0	79
92	The accuracy of local MP2 methods for conformational energies. Molecular Physics, 2008, 106, 1899-1906.	1.7	29
93	Correlation regions within a localized molecular orbital approach. Journal of Chemical Physics, 2008, 128, 144106.	3.0	76
94	Local correlation methods with a natural localized molecular orbital basis. Molecular Physics, 2007, 105, 2753-2761.	1.7	83
95	High-Accuracy Computation of Reaction Barriers in Enzymes. Angewandte Chemie - International Edition, 2006, 45, 6856-6859.	13.8	253
96	Calculation of smooth potential energy surfaces using local electron correlation methods. Journal of Chemical Physics, 2006, 125, 184110.	3.0	82
97	Comparative calculations for the A-frame molecules [S(MPH3)2] (M=Cu, Ag, Au) at levels up to CCSD(T). Chemical Physics Letters, 2005, 405, 148-152.	2.6	38
98	Structural, energetic, and electronic properties of (CH3CN)2â€“8 clusters by density functional theory. Computational and Theoretical Chemistry, 2004, 673, 155-164.	1.5	31
99	NFDI4Chem - Towards a National Research Data Infrastructure for Chemistry in Germany. Research Ideas and Outcomes, 0, 6, .	1.0	25