

# 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	High-Accuracy Computation of Reaction Barriers in Enzymes. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 6856-6859.	13.8	253
2	The inhibition mechanism of human 20 <i>S</i> proteasomes enables next-generation inhibitor design. <i>Science</i> , 2016, 353, 594-598.	12.6	170
3	Benchmarking Quantum Chemical Methods: Are We Heading in the Right Direction?. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 11011-11018.	13.8	119
4	Preparation of $R\text{Sn}(\text{I})\text{Sn}(\text{I})\text{R}$ with Two Unsymmetrically Coordinated Sn(I) Atoms and Subsequent Gentle Activation of $\text{P}^{\text{IV}}$ . <i>Journal of the American Chemical Society</i> , 2011, 133, 17889-17894.	13.7	105
5	The Last Globally Stable Extended Alkane. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 463-466.	13.8	105
6	Manganese(I)-Catalyzed Dispersion-Enabled $\text{C}^{\text{H}}/\text{C}^{\text{C}}$ Activation. <i>Chemistry - A European Journal</i> , 2017, 23, 5443-5447.	3.3	98
7	Local correlation methods with a natural localized molecular orbital basis. <i>Molecular Physics</i> , 2007, 105, 2753-2761.	1.7	83
8	Calculation of smooth potential energy surfaces using local electron correlation methods. <i>Journal of Chemical Physics</i> , 2006, 125, 184110.	3.0	82
9	Does DFT-D estimate accurate energies for the binding of ligands to metal complexes?. <i>Dalton Transactions</i> , 2011, 40, 11176.	3.3	81
10	Toward accurate barriers for enzymatic reactions: QM/MM case study on p-hydroxybenzoate hydroxylase. <i>Journal of Chemical Physics</i> , 2008, 128, 025104.	3.0	79
11	Correlation regions within a localized molecular orbital approach. <i>Journal of Chemical Physics</i> , 2008, 128, 144106.	3.0	76
12	A lysine-cysteine redox switch with an NOS bridge regulates enzyme function. <i>Nature</i> , 2021, 593, 460-464.	27.8	74
13	Free-energy perturbation and quantum mechanical study of SAMPL4 octa-acid host-guest binding energies. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 375-400.	2.9	70
14	Low-barrier hydrogen bonds in enzyme cooperativity. <i>Nature</i> , 2019, 573, 609-613.	27.8	68
15	Solution Structures of Hauser Base $\text{Pr}^{\text{II}}\text{NMgCl}$ and Turbo-Hauser Base $\text{Pr}^{\text{II}}\text{NMgCl}\cdot\text{LiCl}$ in THF and the Influence of LiCl on the Schlenk-Equilibrium. <i>Journal of the American Chemical Society</i> , 2016, 138, 4796-4806.	13.7	65
16	Functional Model for the [Fe] Hydrogenase Inspired by the Frustrated Lewis Pair Concept. <i>Journal of the American Chemical Society</i> , 2014, 136, 16626-16634.	13.7	63
17	Internal dynamics and guest binding of a sterically overcrowded host. <i>Chemical Science</i> , 2016, 7, 4676-4684.	7.4	54
18	Monomeric Sn(II) and Ge(II) hydrides supported by a tridentate pincer-based ligand. <i>Chemical Communications</i> , 2012, 48, 4890.	4.1	53

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19	Limits of Coupled-Cluster Calculations for Non-Heme Iron Complexes. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 922-937.	5.3	51
20	Dinuclear Rhenium Complex with a Proton Responsive Ligand as a Redox Catalyst for the Electrochemical CO <sub>2</sub> Reduction. <i>Inorganic Chemistry</i> , 2017, 56, 4176-4185.	4.0	50
21	An incremental correlation approach to excited state energies based on natural transition/localized orbitals. <i>Journal of Chemical Physics</i> , 2011, 134, 034122.	3.0	47
22	The furan microsolvation blind challenge for quantum chemical methods: First steps. <i>Journal of Chemical Physics</i> , 2018, 148, 014301.	3.0	44
23	Large Density-Functional and Basis-Set Effects for the DMSO Reductase Catalyzed Oxo-Transfer Reaction. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1799-1807.	5.3	42
24	Comparative calculations for the A-frame molecules [S(MPH <sub>3</sub> ) <sub>2</sub> ] (M=Cu, Ag, Au) at levels up to CCSD(T). <i>Chemical Physics Letters</i> , 2005, 405, 148-152.	2.6	38
25	Study of ligand effects in aurophilic interactions using local correlation methods. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 18115.	2.8	37
26	Visualizing dispersion interactions through the use of local orbital spaces. <i>Journal of Computational Chemistry</i> , 2017, 38, 15-23.	3.3	37
27	Pairwise H <sub>2</sub> /D <sub>2</sub> Exchange and H <sub>2</sub> Substitution at a Bimetallic Dinickel(II) Complex Featuring Two Terminal Hydrides. <i>Journal of the American Chemical Society</i> , 2017, 139, 16720-16731.	13.7	36
28	A Stable Cation of a CSi <sub>3</sub> P Five-Membered Ring with a Weakly Coordinating Chloride Anion. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 12510-12513.	13.8	35
29	Widespread occurrence of covalent lysine-cysteine redox switches in proteins. <i>Nature Chemical Biology</i> , 2022, 18, 368-375.	8.0	34
30	Reductive half-reaction of aldehyde oxidoreductase toward acetaldehyde: Ab initio and free energy quantum mechanical/molecular mechanical calculations. <i>Journal of Chemical Physics</i> , 2010, 132, 035101.	3.0	33
31	Structural, energetic, and electronic properties of (CH <sub>3</sub> CN) <sub>2</sub> <sup>8</sup> clusters by density functional theory. <i>Computational and Theoretical Chemistry</i> , 2004, 673, 155-164.	1.5	31
32	Relative anion binding affinity in a series of interpenetrated coordination cages. <i>Dalton Transactions</i> , 2013, 42, 15906.	3.3	31
33	A Simple One-Body Approach to the Calculation of the First Electronic Absorption Band of Water. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1829-1837.	5.3	30
34	The accuracy of local MP2 methods for conformational energies. <i>Molecular Physics</i> , 2008, 106, 1899-1906.	1.7	29
35	Communication: Towards the binding energy and vibrational red shift of the simplest organic hydrogen bond: Harmonic constraints for methanol dimer. <i>Journal of Chemical Physics</i> , 2014, 141, 101105.	3.0	28
36	The first microsolvation step for furans: New experiments and benchmarking strategies. <i>Journal of Chemical Physics</i> , 2020, 152, 164303.	3.0	28

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37	Heteroaromaticity approached by charge density investigations and electronic structure calculations. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 20600.	2.8	27
38	Preorganized Anion Traps for Exploiting Anion- $\pi$ Interactions: An Experimental and Computational Study. <i>Chemistry - A European Journal</i> , 2013, 19, 16988-17000.	3.3	27
39	Influence of size, shape, heteroatom content and dispersive contributions on guest binding in a coordination cage. <i>Chemical Communications</i> , 2017, 53, 11933-11936.	4.1	27
40	Soft hydrogen bonds to alkenes: the methanol-ethene prototype under experimental and theoretical scrutiny. <i>Chemical Science</i> , 2015, 6, 3738-3745.	7.4	26
41	All That Binds Is Not Gold- $\pi$ : The Relative Weight of Auophilic Interactions in Complex Formation. <i>Journal of Physical Chemistry A</i> , 2018, 122, 6918-6925.	2.5	26
42	Structural diversity in sodium doped water trimers. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 9054.	2.8	25
43	NFDI4Chem - Towards a National Research Data Infrastructure for Chemistry in Germany. <i>Research Ideas and Outcomes</i> , 0, 6, .	1.0	25
44	Dynamic polarizability, Cauchy moments, and the optical absorption spectrum of liquid water: A sequential molecular dynamics/quantum mechanical approach. <i>Journal of Chemical Physics</i> , 2009, 130, 014505.	3.0	24
45	Synthesis and Structural Characterization of Homochiral Homo-oligomers of Parent <i>cis</i> - and <i>trans</i> -Furanoid <sup>2</sup> -Amino Acids. <i>Chemistry - A European Journal</i> , 2011, 17, 12946-12954.	3.3	24
46	Highly selective and sensitive fluorescence detection of Zn <sup>2+</sup> and Cd <sup>2+</sup> ions by using an acridine sensor. <i>Dalton Transactions</i> , 2016, 45, 5689-5699.	3.3	24
47	Effects of Metal Coordination on the $\pi$ -System of the 2,5-Bis-((pyrrolidino)-methyl)-pyrrole Pincer Ligand. <i>Inorganic Chemistry</i> , 2013, 52, 9539-9548.	4.0	23
48	A quantum-mechanical study of the reaction mechanism of sulfite oxidase. <i>Journal of Biological Inorganic Chemistry</i> , 2014, 19, 1165-1179.	2.6	23
49	A Computational Comparison of Oxygen Atom Transfer Catalyzed by Dimethyl Sulfide Reductase with Mo and W. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 3580-3589.	2.0	23
50	A push-and-pull model for allosteric anion binding in cage complexes. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 12746.	2.8	22
51	Reaction of $\pi$ -Heterocyclic Silylenes with Thioketone: Formation of Silicon-Sulfur Three (Si <sub>3</sub> S) and Five (Si <sub>5</sub> S) Membered Ring Systems. <i>Chemistry - A European Journal</i> , 2013, 19, 3715-3720.	3.3	22
52	QM/MM study of the reaction mechanism of sulfite oxidase. <i>Scientific Reports</i> , 2018, 8, 4684.	3.3	22
53	Incremental expansions for SCF interaction energies: A comparison for hydrogen-bonded clusters. <i>Chemical Physics Letters</i> , 2008, 465, 136-141.	2.6	20
54	Characterization of a Multicomponent Lithium Lithiate from a Combined X-Ray Diffraction, NMR Spectroscopy, and Computational Approach. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 13282-13287.	13.8	20

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55	Application of high level wavefunction methods in quantum mechanics/molecular mechanics hybrid schemes. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 5041.	2.8	18
56	Coupled-Cluster Interaction Energies for 200-Atom Host-Guest Systems. <i>ChemPhysChem</i> , 2014, 15, 3270-3281.	2.1	18
57	Time-Resolved Spectroscopy of Photoinduced Electron Transfer in Dinuclear and Tetranuclear Fe/Co Prussian Blue Analogues. <i>Inorganic Chemistry</i> , 2021, 60, 449-459.	4.0	18
58	Electronic Excitation of Cl <sup>+</sup> in Liquid Water and at the Surface of a Cluster: A Sequential Born-Oppenheimer Molecular Dynamics/Quantum Mechanics Approach. <i>Journal of Physical Chemistry A</i> , 2009, 113, 14684-14690.	2.5	15
59	The Layered Structure of [Na(NH <sub>3</sub> ) <sub>4</sub> ][Indenide] Containing a Square-Planar Na(NH <sub>3</sub> ) <sub>4</sub> <sup>+</sup> Cation. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 734-738.	13.8	15
60	Lipoxygenase 2 from <i>Cyanotheca</i> sp. controls dioxygen insertion by steric shielding and substrate fixation. <i>Scientific Reports</i> , 2017, 7, 2069.	3.3	14
61	Quantenchemische Methoden im Leistungsvergleich: Stimmt die Richtung noch?. <i>Angewandte Chemie</i> , 2017, 129, 11155-11163.	2.0	14
62	Ligand Protonation Triggers H <sub>2</sub> Release from a Dinickel Dihydride Complex to Give a Doubly $\sigma$ -T <sub>g</sub> -Shaped Dinickel(I) Metallodiradical. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 1891-1896.	13.8	13
63	Atomdroid: A Computational Chemistry Tool for Mobile Platforms. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 1072-1078.	5.4	12
64	Strong Intermolecular Interactions Shaping a Small Piano-Stool Complex. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 10365-10369.	13.8	12
65	The phenyl vinyl ether-methanol complex: a model system for quantum chemistry benchmarking. <i>Beilstein Journal of Organic Chemistry</i> , 2018, 14, 1642-1654.	2.2	12
66	In-Fjord Substitution in Expanded Helicenes: Effects of the Insert on the Inversion Barrier and Helical Pitch. <i>Chemistry - A European Journal</i> , 2021, 27, 13358-13366.	3.3	12
67	Ground-state destabilization by electrostatic repulsion is not a driving force in orotidine-5 <sup>2</sup> -monophosphate decarboxylase catalysis. <i>Nature Catalysis</i> , 2022, 5, 332-341.	34.4	12
68	Ein kleiner Klavierstuhl-Komplex, geformt durch starke intermolekulare Wechselwirkungen. <i>Angewandte Chemie</i> , 2013, 125, 10555-10559.	2.0	10
69	Local Hybrid QM/QM Calculations of Reaction Pathways in Metallobiosites. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5397-5404.	5.3	10
70	Theoretical Studies of the Electronic Absorption Spectra of Thiamin Diphosphate in Pyruvate Decarboxylase. <i>Biochemistry</i> , 2017, 56, 1854-1864.	2.5	10
71	Anomeric Stereoauxiliary Cleavage of the C-N Bond of $\alpha$ -Glucosamine for the Preparation of Imidazo[1,5-a]pyridines. <i>Chemistry - A European Journal</i> , 2022, 28, .	3.3	10
72	Strained hydrogen bonding in imidazole trimer: a combined infrared, Raman, and theory study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 5989-5998.	2.8	9

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73	Setting up the HyDRA blind challenge for the microhydration of organic molecules. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 11442-11454.	2.8	9
74	Assessing the accuracy of many-body expansions for the computation of solvatochromic shifts. <i>Molecular Physics</i> , 2010, 108, 381-392.	1.7	8
75	Photoionization of CH <sub>3</sub> N <sub>3</sub> Produces <sup>3</sup> B <sub>2</sub> N <sub>3</sub> <sup>+</sup> : A Theoretical and Experimental Study of the Ion-Pair Channel. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2311-2315.	4.6	8
76	Accelerating the Computation of Induced Dipoles for Molecular Mechanics with Dataflow Engines. , 2013, , .		8
77	Bracketing subtle conformational energy differences between self-solvated and stretched trifluoropropanol. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 9899-9909.	2.8	8
78	A Review of Density Functional Models for the Description of Fe(II) Spin-Crossover Complexes. <i>Molecules</i> , 2020, 25, 5176.	3.8	8
79	Electrophilic Cyanative Alkenylation of Arenes. <i>Organic Letters</i> , 2020, 22, 4932-4937.	4.6	8
80	Photochemical Properties of Re(CO) <sub>3</sub> Complexes with and without a Local Proton Source and Implications for CO <sub>2</sub> Reduction Catalysis. <i>Organometallics</i> , 2020, 39, 2405-2414.	2.3	8
81	Dispersion forces in chirality recognition â€” a density functional and wave function theory study of diols. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 12093-12104.	2.8	8
82	Helium Nanodroplet Study of the Hydrogen-Bonded OH Vibrations in HClâ€”H <sub>2</sub> O Clusters. <i>Journal of Physical Chemistry A</i> , 2015, 119, 2636-2643.	2.5	7
83	Temperatureâ€”Dependent Dynamics of Pushâ€”Pull Rotor Systems Based on Acridinylidene Cyanoacetic Esters. <i>European Journal of Organic Chemistry</i> , 2017, 2017, 5141-5146.	2.4	6
84	Hybrid Local Molecular Orbital: Molecular Orbital Calculations for Open Shell Systems. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5192-5202.	5.3	6
85	A full additive QM/MM scheme for the computation of molecular crystals with extension to many-body expansions. <i>Journal of Chemical Physics</i> , 2019, 150, 154118.	3.0	6
86	Iterative induced dipoles computation for molecular mechanics on GPUs. , 2010, , .		5
87	QM/MM Approaches to the Electronic Spectra of Hydrogen-Bonding Systems with Connection to Many-Body Decomposition Schemes. <i>Advances in Quantum Chemistry</i> , 2010, , 99-144.	0.8	4
88	Study of Specific Ionâ€”Amino Acid Interactions through the Use of Local Correlation Methods. <i>Journal of Physical Chemistry A</i> , 2012, 116, 5464-5471.	2.5	4
89	Application of Local Second-Order MÃ¶llerâ€”Plesset Perturbation Theory to the Study of Structures in Solution. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3053-3060.	5.3	4
90	High level potential energy surface and mechanism of Al(CH <sub>3</sub> ) <sub>2</sub> OCH <sub>3</sub> -promoted lactone polymerization: initiation and propagation. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 8989-8999.	2.8	4

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91	A high-throughput computational approach to UV-Vis spectra in protein mutants. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 20678-20692.	2.8	4
92	Critical Assessment of RAFT Equilibrium Constants: Theory Meets Experiment. <i>Macromolecular Theory and Simulations</i> , 2020, 29, 2000022.	1.4	4
93	Ligand Protonation Triggers H <sub>2</sub> Release from a Dinickel Dihydride Complex to Give a Doubly $\eta^5$ -Shaped Dinickel(I) Metalloradical. <i>Angewandte Chemie</i> , 2021, 133, 1919-1924.	2.0	4
94	Theoretical Studies of the Acid-Base Equilibria in a Model Active Site of the Human 20S Proteasome. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 1942-1953.	5.4	4
95	Computation of Induced Dipoles in Molecular Mechanics Simulations Using Graphics Processors. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 1159-1166.	5.4	3
96	Optimization and benchmarking of a perturbative Metropolis Monte Carlo quantum mechanics/molecular mechanics program. <i>Journal of Chemical Physics</i> , 2017, 147, 244105.	3.0	2
97	Experimental charge density study on FLPs and a FLP reaction product. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2018, 233, 723-731.	0.8	2
98	Efficient parallelization of perturbative Monte Carlo QM/MM simulations in heterogeneous platforms. <i>International Journal of High Performance Computing Applications</i> , 2017, 31, 499-516.	3.7	1
99	FJK - A cap-free fragment approach with embedding Fock potentials. <i>AIP Conference Proceedings</i> , 2015, , .	0.4	0