Ivan Rivalta

List of Publications by Year
in descending order

93	4,326	147566 31	114278 63
papers	citations	h-index	g-index

96	96	96	4944
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. Journal of Computational Chemistry, 2016, 37, 506-541.	1.5	1,317
2	Allostery in Its Many Disguises: From Theory to Applications. Structure, 2019, 27, 566-578.	1.6	285
3	S₁-State Model of the O₂-Evolving Complex of Photosystem II. Biochemistry, 2011, 50, 6308-6311.	1.2	210
4	Allosteric pathways in imidazole glycerol phosphate synthase. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, E1428-36.	3.3	192
5	Eigenvector centrality for characterization of protein allosteric pathways. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E12201-E12208.	3.3	145
6	Structuralâ€“Functional Role of Chloride in Photosystem II. Biochemistry, 2011, 50, 6312-6315.	1.2	132
7	Protospacer Adjacent Motif-Induced Allostery Activates CRISPR-Cas9. Journal of the American Chemical Society, 2017, 139, 16028-16031.	6.6	104
8	Key role of the REC lobe during CRISPRâ€“Cas9 activation by â€˜sensingâ€™, â€˜regulatingâ€™, and â€˜lockingâ€™ the catalytic HNH domain. Quarterly Reviews of Biophysics, 2018, 51, .	2.4	79
9	Oxomanganese complexes for natural and artificial photosynthesis. Current Opinion in Chemical Biology, 2012, 16, 11-18.	2.8	77
10	Characterization of an Amorphous Iridium Water-Oxidation Catalyst Electrodeposited from Organometallic Precursors. Inorganic Chemistry, 2013, 52, 1860-1871.	1.9	65
11	COBRAMM 2.0 â€” A software interface for tailoring molecular electronic structure calculations and running nanoscale (QM/MM) simulations. Journal of Molecular Modeling, 2018, 24, 271.	0.8	55
12	Facile Ecofriendly Synthesis of Monastrol and Its Structural Isomers via Biginelli Reaction. ACS Sustainable Chemistry and Engineering, 2014, 2, 1228-1233.	3.2	50
13	UV-induced long-lived decays in solvated pyrimidine nucleosides resolved at the MS-CASPT2/MM level. Physical Chemistry Chemical Physics, 2018, 20, 6877-6890.	1.3	46
14	Modeling the high-energy electronic state manifold of adenine: Calibration for nonlinear electronic spectroscopy. Journal of Chemical Physics, 2015, 142, 212443.	1.2	44
15	Solution NMR and Computational Methods for Understanding Protein Allostery. Journal of Physical Chemistry B, 2013, 117, 3063-3073.	1.2	40
16	Two-dimensional UV spectroscopy: a new insight into the structure and dynamics of biomolecules. Chemical Science, 2019, 10, 9907-9921.	3.7	40
17	Spectral lineshapes in nonlinear electronic spectroscopy. Physical Chemistry Chemical Physics, 2015, 17, 30925-30936.	1.3	39
18	Allosteric Pathways in the PPARÎ³-RXRÎ± nuclear receptor complex. Scientific Reports, 2016, 6, 19940.	1.6	39

#	Article	IF	Citations
19	Ab initio simulations of two-dimensional electronic spectra: The SOS//QM/MM approach. International Journal of Quantum Chemistry, 2014, 114, 85-93.	1.0	38
20	Dissecting Dynamic Allosteric Pathways Using Chemically Related Small-Molecule Activators. Structure, 2016, 24, 1155-1166.	1.6	38
21	The role of quantum chemistry in the elucidation of the elementary mechanisms of catalytic processes: from atoms, to surfaces, to enzymes. Theoretical Chemistry Accounts, 2007, 117, 765-779.	0.5	37
22	Acetylene Cyclotrimerization by Early Second-Row Transition Metals in the Gas Phase. A Theoretical Study. Inorganic Chemistry, 2005, 44, 9807-9816.	1.9	36
23	Interaction of CO with PdAu(111) and PdAu(100) Bimetallic Surfaces:â€‰ A Theoretical Cluster Model Study. Journal of Physical Chemistry C, 2008, 112, 6073-6081.	1.5	36
24	Electrostatic Effects on Proton Coupled Electron Transfer in Oxomanganese Complexes Inspired by the Oxygen-Evolving Complex of Photosystem II. Journal of Physical Chemistry B, 2013, 117, 6217-6226.	1.2	36
25	Modelling Time-Resolved Two-Dimensional Electronic Spectroscopy of the Primary Photoisomerization Event in Rhodopsin. Journal of Physical Chemistry B, 2014, 118, 8396-8405.	1.2	35
26	Excited state evolution of DNA stacked adenines resolved at the CASPT2//CASSCF/Amber level: from the bright to the excimer state and back. Physical Chemistry Chemical Physics, 2015, 17, 7291-7302.	1.3	35
27	Tracking the primary photoconversion events in rhodopsins by ultrafast optical spectroscopy. Photochemical and Photobiological Sciences, 2015, 14, 213-228.	1.6	35
28	Decrypting the Information Exchange Pathways across the Spliceosome Machinery. Journal of the American Chemical Society, 2020, 142, 8403-8411.	6.6	35
29	Disentangling Peptide Configurations via Two-Dimensional Electronic Spectroscopy: Ab Initio Simulations Beyond the Frenkel Exciton Hamiltonian. Journal of Physical Chemistry Letters, 2014, 5, 767-771.	2.1	34
30	Methane activation by chromium oxide cations in the gas phase: A theoretical study. Journal of Computational Chemistry, 2006, 27, 174-187.	1.5	33
31	Modelling retinal chromophores photoisomerization: from minimal models in vacuo to ultimate bidimensional spectroscopy in rhodopsins. Physical Chemistry Chemical Physics, 2014, 16, 16865-16879.	1.3	33
32	Allosteric Communication Disrupted by a Small Molecule Binding to the Imidazole Glycerol Phosphate Synthase Proteinâ€“Protein Interface. Biochemistry, 2016, 55, 6484-6494.	1.2	33
33	Tracking excited state decay mechanisms of pyrimidine nucleosides in real time. Nature Communications, 2021, 12, 7285.	5.8	32
34	Deciphering the photochemical mechanisms describing the UV-induced processes occurring in solvated guanine monophosphate. Frontiers in Chemistry, 2015, 3, 29.	1.8	31
35	Multiple Decay Mechanisms and 2Dâ€UV Spectroscopic Fingerprints of Singlet Excited Solvated Adenineâ€Uracil Monophosphate. Chemistry - A European Journal, 2016, 22, 7497-7507.	1.7	31
36	Noncollinear Spins Provide a Self-Consistent Treatment of the Low-Spin State of a Biomimetic Oxomanganese Synthetic Trimer Inspired by the Oxygen Evolving Complex of Photosystem II. Journal of Physical Chemistry Letters, 2011, 2, 2629-2633.	2.1	29

#	Article	IF	Citations
37	Probing deactivation pathways of DNA nucleobases by two-dimensional electronic spectroscopy: first principles simulations. Faraday Discussions, 2015, 177, 345-362.	1.6	29
38	Exploring Allosteric Pathways of a V-Type Enzyme with Dynamical Perturbation Networks. Journal of Physical Chemistry B, 2019, 123, 3452-3461.	1.2	29
39	Adsorption of Ethylene, Vinyl, Acetic Acid, and Acetate Species on PdAu(111) and PdAu(100) Surface Alloys: A Cluster Model Study. Journal of Chemical Theory and Computation, 2009, 5, 1350-1360.	2.3	28
40	Reengineering Rate-Limiting, Millisecond Enzyme Motions by Introduction of an Unnatural Amino Acid. Biophysical Journal, 2011, 101, 411-420.	0.2	28
41	Spectroscopic fingerprints of DNA/RNA pyrimidine nucleobases in third-order nonlinear electronic spectra. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	28
42	Two-Dimensional Electronic Spectroscopy of Benzene, Phenol, and Their Dimer: An Efficient First-Principles Simulation Protocol. Journal of Chemical Theory and Computation, 2015, 11, 3755-3771.	2.3	27
43	On the insertion mechanism of molecular oxygen into a Pd(II)â€“H bond. Something to add. Chemical Physics Letters, 2007, 443, 183-189.	1.2	25
44	Insight on Chirality Encoding from Small Thiolated Molecule to Plasmonic Au@Ag and Au@Au Nanoparticles. ACS Nano, 2022, 16, 1089-1101.	7.3	25
45	Activation of Methane by the Iron Dimer Cation. A Theoretical Study. Journal of Physical Chemistry A, 2006, 110, 12501-12511.	1.1	24
46	Spectral Tuning of Ultraviolet Cone Pigments: An Interhelical Lock Mechanism. Journal of the American Chemical Society, 2013, 135, 19064-19067.	6.6	24
47	Modeling multidimensional spectral lineshapes from first principles: application to water-solvated adenine. Faraday Discussions, 2019, 221, 219-244.	1.6	24
48	Atomic configurations of Pd atoms in PdAu(111) and PdAu(100) surface alloys: Ab initio density functional calculations. Chemical Physics Letters, 2009, 468, 162-165.	1.2	23
49	Tracking Conformational Dynamics of Polypeptides by Nonlinear Electronic Spectroscopy of Aromatic Residues: A Firstâ€Principles Simulation Study. ChemPhysChem, 2014, 15, 3282-3290.	1.0	23
50	Fine Tuning of Retinal Photoinduced Decay in Solution. Journal of Physical Chemistry Letters, 2017, 8, 4407-4412.	2.1	23
51	Towards Accurate Simulation of Two-Dimensional Electronic Spectroscopy. Topics in Current Chemistry, 2018, 376, 24.	3.0	23
52	Theoretical Investigation of the Mechanism of Acid-Catalyzed Oxygenation of a Pd(II)-Hydride To Produce a Pd(II)-Hydroperoxide. Journal of Chemical Theory and Computation, 2008, 4, 1283-1292.	2.3	21
53	Bidimensional electronic spectroscopy on indole in gas phase and in water from first principles. Computational and Theoretical Chemistry, 2014, 1040-1041, 295-303.	1.1	21
54	Boosting the guerbet reaction: A cooperative catalytic system for the efficient bio-ethanol refinery to second-generation biofuels. Journal of Catalysis, 2022, 405, 47-59.	3.1	19

#	Article	IF	Citations
55	Characterization of Protein Tyrosine Phosphatase 1B Inhibition by Chlorogenic Acid and Cichoric Acid. Biochemistry, 2017, 56, 96-106.	1.2	18
56	Resolving the Singlet Excited State Manifold of Benzophenone by First-Principles Simulations and Ultrafast Spectroscopy. Journal of Chemical Theory and Computation, 2018, 14, 2570-2585.	2.3	16
57	The recognition of a new pathway for the reaction of molecular oxygen with a Pd(II)-hydride to produce a Pd(II)-hydroperoxide. Chemical Physics Letters, 2008, 456, 41-46.	1.2	15
58	The geometric effect in palladiumâ€“gold catalysis. Is the coupling the rate-determining step in the vinyl-acetate synthesis?. Chemical Communications, 2009, , 1852.	2.2	15
59	Triplet Oxygen Evolution Catalyzed by a Biomimetic Oxomanganese Complex: Functional Role of the Carboxylate Buffer. ACS Catalysis, 2015, 5, 2384-2390.	5.5	15
60	Simulating Plasmon Resonances of Gold Nanoparticles with Bipyramidal Shapes by Boundary Element Methods. Journal of Chemical Theory and Computation, 2020, 16, 3807-3815.	2.3	15
61	Community Network Analysis of Allosteric Proteins. Methods in Molecular Biology, 2021, 2253, 137-151.	0.4	15
62	A theoretical study of ethylene dehydrogenation by bare Niobium atom and cation. Computational and Theoretical Chemistry, 2006, 762, 25-31.	1.5	14
63	The highly excited-state manifold of guanine: calibration for nonlinear electronic spectroscopy simulations. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	14
64	Two-dimensional electronic spectroscopy as a tool for tracking molecular conformations in DNA/RNA aggregates. Faraday Discussions, 2018, 207, 233-250.	1.6	14
65	First-principles characterization of the singlet excited state manifold in DNA/RNA nucleobases. Physical Chemistry Chemical Physics, 2020, 22, 15496-15508.	1.3	14
66	Sodium diffusion in ionic liquid-based electrolytes for Na-ion batteries: the effect of polarizable force fields. Physical Chemistry Chemical Physics, 2020, 22, 20114-20122.	1.3	13
67	The influence of surface oxygen and hydroxyl groups on the dehydrogenation of ethylene on PdAu surface alloys. A theoretical cluster model study. Chemical Physics Letters, 2010, 493, 87-93.	1.2	11
68	The effect of solvent relaxation in the ultrafast time-resolved spectroscopy of solvated benzophenone. Photochemical and Photobiological Sciences, 2018, 17, 323-331.	1.6	10
69	Bimetallic Coâ€“M (M = Cu, Ag, and Au) Carbonyl Complexes Supported by N-Heterocyclic Carbene Ligands: Synthesis, Structures, Computational Investigation, and Catalysis for Ammonia Borane Dehydrogenation. Organometallics, 2021, 40, 2724-2735.	1.1	10
70	Theoretical study of the gas-phase ethane Câ€“H and Câ€“C bonds activation by bare niobium cation. Theoretical Chemistry Accounts, 2008, 120, 395-403.	0.5	9
71	Control of Protonated Schiff Base Excited State Decay within Visual Protein Mimics: A Unified Model for Retinal Chromophores. Chemistry - A European Journal, 2021, 27, 16389-16400.	1.7	9
72	Theoretical Model of the Protochlorophyllide Oxidoreductase from a Hierarchy of Protocols. Journal of Physical Chemistry B, 2018, 122, 7668-7681.	1.2	8

#	Article	IF	Citations
73	Distinct allosteric pathways in imidazole glycerol phosphate synthase from yeast and bacteria. Biophysical Journal, 2022, 121, 119-130.	0.2	8
74	Pd, Rh, Ir and Pt adsorption on gold: A theoretical study of different surfaces. Chemical Physics Letters, 2007, 442, 105-109.	1.2	6
75	Detecting Dissociation Dynamics of Phosphorus Molecular Ions by Atom Probe Tomography. Journal of Physical Chemistry A, 2020, 124, 10977-10988.	1.1	6
76	Heterometallic rhodium clusters as electron reservoirs: Chemical, electrochemical, and theoretical studies of the centered-icosahedral [Rh12E(CO)27]nâ^' atomically precise carbonyl compounds. Journal of Chemical Physics, 2021, 155, 104301.	1.2	6
77	Ultraviolet vision: photophysical properties of the unprotonated retinyl Schiff base in the Siberian hamster cone pigment. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	5
78	On the origin of controlled anisotropic growth of monodisperse gold nanobipyramids. Nanoscale, 2021, 13, 15292-15300.	2.8	5
79	Singular Interface Dynamics of the SARS-CoV-2 Delta Variant Explained with Contact Perturbation Analysis. Journal of Chemical Information and Modeling, 2022, 62, 3107-3122.	2.5	5
80	Towards Accurate Simulation of Two-Dimensional Electronic Spectroscopy. Topics in Current Chemistry Collections, 2019, , 63-112.	0.2	4
81	Polymerization Isomerism in Co-M (M = Cu, Ag, Au) Carbonyl Clusters: Synthesis, Structures and Computational Investigation. Molecules, 2021, 26, 1529.	1.7	4
82	Photo-Active Biological Molecular Materials: From Photoinduced Dynamics to Transient Electronic Spectroscopies. Challenges and Advances in Computational Chemistry and Physics, 2021, , 77-142.	0.6	4
83	Soft X-ray Spectroscopic Properties of Ruthenium Complex Catalyst under CO₂ Electrochemical Reduction Conditions: A First-Principles Study. Journal of Physical Chemistry C, 2015, 119, 22899-22907.	1.5	3
84	Ternary Complex Formation and Photoactivation of a Photoenzyme Results in Altered Protein Dynamics. Journal of Physical Chemistry B, 2019, 123, 7372-7384.	1.2	3
85	Carbon dioxide reduction mechanism on Ru-based electrocatalysts [Ru(bpy)₂(CO)₂]²⁺: insights from first-principles theory. Sustainable Energy and Fuels, 2021, 5, 6066-6076.	2.5	3
86	Ultrafast Carotenoid to Retinal Energy Transfer in Xanthorhodopsin Revealed by the Combination of Transient Absorption and Twoâ€Dimensional Electronic Spectroscopy. Chemistry - A European Journal, 2018, 24, 12084-12092.	1.7	2
87	Computational Studies of the Oxygen-Evolving Complex of Photosystem II and Biomimetic Oxomanganese Complexes for Renewable Energy Applications. ACS Symposium Series, 2013, , 203-215.	0.5	1
88	An Allosteric Signaling Governs the CRISPR-Cas9 Function. Biophysical Journal, 2019, 116, 485a.	0.2	1
89	Elucidating the Activation Mechanism of AMPK by Direct Pan-Activator PF-739. Frontiers in Molecular Biosciences, 2021, 8, 760026.	1.6	1
90	Modelling quenching mechanisms of disordered molecular systems in the presence of molecular aggregates. Physical Chemistry Chemical Physics, 2022, 24, 1787-1794.	1.3	1

#	Article	IF	Citations
91	Activation of a Photoenzyme Results in Modified Structure and Dynamics. Biophysical Journal, 2020, 118, 192a-193a.	0.2	0
92	TOWARD THE ACCURATE SIMULATION OF TWO-DIMENSIONAL ELECTRONIC SPECTRA. , 2015, , .		0
93	Two-State Reaction Paradigm in Transition Metals Mediated Reactions. , 2019, , 1115-1118.		0