

Ivan Rivalta

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

89
papers

3,242
citations

27
h-index

55
g-index

96
ext. papers

3,837
ext. citations

4.8
avg, IF

4.97
L-index

#	Paper	IF	Citations
89	Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. <i>Journal of Computational Chemistry</i> , 2016 , 37, 506-41	3.5	1047
88	S1-state model of the O ₂ -evolving complex of photosystem II. <i>Biochemistry</i> , 2011 , 50, 6308-11	3.2	196
87	Allostery in Its Many Disguises: From Theory to Applications. <i>Structure</i> , 2019 , 27, 566-578	5.2	158
86	Allosteric pathways in imidazole glycerol phosphate synthase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012 , 109, E1428-36	11.5	142
85	Structural-functional role of chloride in photosystem II. <i>Biochemistry</i> , 2011 , 50, 6312-5	3.2	114
84	Oxomanganese complexes for natural and artificial photosynthesis. <i>Current Opinion in Chemical Biology</i> , 2012 , 16, 11-8	9.7	73
83	Eigenvector centrality for characterization of protein allosteric pathways. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, E12201-E12208	11.5	72
82	Protospacer Adjacent Motif-Induced Allostery Activates CRISPR-Cas9. <i>Journal of the American Chemical Society</i> , 2017 , 139, 16028-16031	16.4	66
81	Characterization of an amorphous iridium water-oxidation catalyst electrodeposited from organometallic precursors. <i>Inorganic Chemistry</i> , 2013 , 52, 1860-71	5.1	59
80	Facile Ecofriendly Synthesis of Monastrol and Its Structural Isomers via Biginelli Reaction. <i>ACS Sustainable Chemistry and Engineering</i> , 2014 , 2, 1228-1233	8.3	44
79	Key role of the REC lobe during CRISPR-Cas9 activation by Sensing, Regulating, and Docking the catalytic HNH domain. <i>Quarterly Reviews of Biophysics</i> , 2018 , 51,	7	42
78	Modeling the high-energy electronic state manifold of adenine: Calibration for nonlinear electronic spectroscopy. <i>Journal of Chemical Physics</i> , 2015 , 142, 212443	3.9	37
77	The role of quantum chemistry in the elucidation of the elementary mechanisms of catalytic processes: from atoms, to surfaces, to enzymes. <i>Theoretical Chemistry Accounts</i> , 2007 , 117, 765-779	1.9	36
76	Solution NMR and computational methods for understanding protein allostery. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 3063-73	3.4	35
75	Interaction of CO with PdAu(111) and PdAu(100) Bimetallic Surfaces: A Theoretical Cluster Model Study. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 6073-6081	3.8	35
74	Spectral lineshapes in nonlinear electronic spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 30925-36	3.6	34
73	Ab initio simulations of two-dimensional electronic spectra: The SOS//QM/MM approach. <i>International Journal of Quantum Chemistry</i> , 2014 , 114, 85-93	2.1	34

72	UV-induced long-lived decays in solvated pyrimidine nucleosides resolved at the MS-CASPT2/MM level. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 6877-6890	3.6	32
71	Electrostatic effects on proton coupled electron transfer in oxomanganese complexes inspired by the oxygen-evolving complex of photosystem II. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 6217-26	3.4	32
70	Excited state evolution of DNA stacked adenines resolved at the CASPT2//CASSCF/Amber level: from the bright to the excimer state and back. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 7291-302	3.6	31
69	Disentangling Peptide Configurations via Two-Dimensional Electronic Spectroscopy: Ab Initio Simulations Beyond the Frenkel Exciton Hamiltonian. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 767-771	6.4	31
68	Allosteric Pathways in the PPAR α nuclear receptor complex. <i>Scientific Reports</i> , 2016 , 6, 19940	4.9	31
67	Modelling retinal chromophores photoisomerization: from minimal models in vacuo to ultimate bidimensional spectroscopy in rhodopsins. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 16865-79	3.6	30
66	Methane activation by chromium oxide cations in the gas phase: a theoretical study. <i>Journal of Computational Chemistry</i> , 2006 , 27, 174-87	3.5	30
65	Dissecting Dynamic Allosteric Pathways Using Chemically Related Small-Molecule Activators. <i>Structure</i> , 2016 , 24, 1155-66	5.2	29
64	COBRAMM 2.0 - A software interface for tailoring molecular electronic structure calculations and running nanoscale (QM/MM) simulations. <i>Journal of Molecular Modeling</i> , 2018 , 24, 271	2	29
63	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. <i>Journal of Physical Chemistry Letters</i> , 2011 , 2, 2629-2633	6.4	28
62	Tracking the primary photoconversion events in rhodopsins by ultrafast optical spectroscopy. <i>Photochemical and Photobiological Sciences</i> , 2015 , 14, 213-28	4.2	27
61	Probing deactivation pathways of DNA nucleobases by two-dimensional electronic spectroscopy: first principles simulations. <i>Faraday Discussions</i> , 2015 , 177, 345-62	3.6	27
60	Modelling time-resolved two-dimensional electronic spectroscopy of the primary photoisomerization event in rhodopsin. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 8396-405	3.4	27
59	Multiple Decay Mechanisms and 2D-UV Spectroscopic Fingerprints of Singlet Excited Solvated Adenine-Uracil Monophosphate. <i>Chemistry - A European Journal</i> , 2016 , 22, 7497-507	4.8	26
58	Acetylene cyclotrimerization by early second-row transition metals in the gas phase. A theoretical study. <i>Inorganic Chemistry</i> , 2005 , 44, 9807-16	5.1	26
57	Allosteric Communication Disrupted by a Small Molecule Binding to the Imidazole Glycerol Phosphate Synthase Protein-Protein Interface. <i>Biochemistry</i> , 2016 , 55, 6484-6494	3.2	25
56	On the insertion mechanism of molecular oxygen into a Pd(II) bond. Something to add. <i>Chemical Physics Letters</i> , 2007 , 443, 183-189	2.5	24
55	Spectroscopic fingerprints of DNA/RNA pyrimidine nucleobases in third-order nonlinear electronic spectra. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	24

54	Two-dimensional UV spectroscopy: a new insight into the structure and dynamics of biomolecules. <i>Chemical Science</i> , 2019 , 10, 9907-9921	9.4	24
53	Two-Dimensional Electronic Spectroscopy of Benzene, Phenol, and Their Dimer: An Efficient First-Principles Simulation Protocol. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 3755-71	6.4	23
52	Deciphering the photochemical mechanisms describing the UV-induced processes occurring in solvated guanine monophosphate. <i>Frontiers in Chemistry</i> , 2015 , 3, 29	5	23
51	Adsorption of Ethylene, Vinyl, Acetic Acid, and Acetate Species on PdAu(111) and PdAu(100) Surface Alloys: A Cluster Model Study. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 1350-60	6.4	23
50	Activation of methane by the iron dimer cation. A theoretical study. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 12501-11	2.8	23
49	Tracking conformational dynamics of polypeptides by nonlinear electronic spectroscopy of aromatic residues: a first-principles simulation study. <i>ChemPhysChem</i> , 2014 , 15, 3282-90	3.2	22
48	Theoretical Investigation of the Mechanism of Acid-Catalyzed Oxygenation of a Pd(II)-Hydride To Produce a Pd(II)-Hydroperoxide. <i>Journal of Chemical Theory and Computation</i> , 2008 , 4, 1283-92	6.4	21
47	Bidimensional electronic spectroscopy on indole in gas phase and in water from first principles. <i>Computational and Theoretical Chemistry</i> , 2014 , 1040-1041, 295-303	2	20
46	Spectral tuning of ultraviolet cone pigments: an interhelical lock mechanism. <i>Journal of the American Chemical Society</i> , 2013 , 135, 19064-7	16.4	20
45	Atomic configurations of Pd atoms in PdAu(111) and PdAu(100) surface alloys: Ab initio density functional calculations. <i>Chemical Physics Letters</i> , 2009 , 468, 162-165	2.5	20
44	Modeling multidimensional spectral lineshapes from first principles: application to water-solvated adenine. <i>Faraday Discussions</i> , 2019 , 221, 219-244	3.6	17
43	Towards Accurate Simulation of Two-Dimensional Electronic Spectroscopy. <i>Topics in Current Chemistry</i> , 2018 , 376, 24	7.2	16
42	The recognition of a new pathway for the reaction of molecular oxygen with a Pd(II)-hydride to produce a Pd(II)-hydroperoxide. <i>Chemical Physics Letters</i> , 2008 , 456, 41-46	2.5	15
41	Characterization of Protein Tyrosine Phosphatase 1B Inhibition by Chlorogenic Acid and Cichoric Acid. <i>Biochemistry</i> , 2017 , 56, 96-106	3.2	14
40	Exploring Allosteric Pathways of a V-Type Enzyme with Dynamical Perturbation Networks. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 3452-3461	3.4	14
39	Triplet Oxygen Evolution Catalyzed by a Biomimetic Oxomanganese Complex: Functional Role of the Carboxylate Buffer. <i>ACS Catalysis</i> , 2015 , 5, 2384-2390	13.1	14
38	Fine Tuning of Retinal Photoinduced Decay in Solution. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 4407-4412	6.4	14
37	The geometric effect in palladium-gold catalysis. Is the coupling the rate-determining step in the vinyl-acetate synthesis?. <i>Chemical Communications</i> , 2009 , 1852-4	5.8	14

36	A theoretical study of ethylene dehydrogenation by bare Niobium atom and cation. <i>Computational and Theoretical Chemistry</i> , 2006 , 762, 25-31		14
35	Decrypting the Information Exchange Pathways across the Spliceosome Machinery. <i>Journal of the American Chemical Society</i> , 2020 , 142, 8403-8411	16.4	13
34	Reengineering rate-limiting, millisecond enzyme motions by introduction of an unnatural amino acid. <i>Biophysical Journal</i> , 2011 , 101, 411-20	2.9	13
33	Resolving the Singlet Excited State Manifold of Benzophenone by First-Principles Simulations and Ultrafast Spectroscopy. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 2570-2585	6.4	12
32	The highly excited-state manifold of guanine: calibration for nonlinear electronic spectroscopy simulations. <i>Theoretical Chemistry Accounts</i> , 2018 , 137, 1	1.9	10
31	Two-dimensional electronic spectroscopy as a tool for tracking molecular conformations in DNA/RNA aggregates. <i>Faraday Discussions</i> , 2018 , 207, 233-250	3.6	10
30	Simulating Plasmon Resonances of Gold Nanoparticles with Bipyramidal Shapes by Boundary Element Methods. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 3807-3815	6.4	9
29	The effect of solvent relaxation in the ultrafast time-resolved spectroscopy of solvated benzophenone. <i>Photochemical and Photobiological Sciences</i> , 2018 , 17, 323-331	4.2	8
28	Theoretical study of the gas-phase ethane C-H and C-C bonds activation by bare niobium cation. <i>Theoretical Chemistry Accounts</i> , 2008 , 120, 395-403	1.9	8
27	Community Network Analysis of Allosteric Proteins. <i>Methods in Molecular Biology</i> , 2021 , 2253, 137-151	1.4	8
26	Theoretical Model of the Protochlorophyllide Oxidoreductase from a Hierarchy of Protocols. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 7668-7681	3.4	7
25	First-principles characterization of the singlet excited state manifold in DNA/RNA nucleobases. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 15496-15508	3.6	6
24	The influence of surface oxygen and hydroxyl groups on the dehydrogenation of ethylene on PdAu surface alloys. A theoretical cluster model study. <i>Chemical Physics Letters</i> , 2010 , 493, 87-93	2.5	5
23	Pd, Rh, Ir and Pt adsorption on gold: A theoretical study of different surfaces. <i>Chemical Physics Letters</i> , 2007 , 442, 105-109	2.5	5
22	Detecting Dissociation Dynamics of Phosphorus Molecular Ions by Atom Probe Tomography. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 10977-10988	2.8	4
21	Ultraviolet vision: photophysical properties of the unprotonated retinyl Schiff base in the Siberian hamster cone pigment. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	4
20	Tracking excited state decay mechanisms of pyrimidine nucleosides in real time		3
19	Sodium diffusion in ionic liquid-based electrolytes for Na-ion batteries: the effect of polarizable force fields. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 20114-20122	3.6	3

18	Towards Accurate Simulation of Two-Dimensional Electronic Spectroscopy. <i>Topics in Current Chemistry Collections</i> , 2019 , 63-112	1.8	3
17	Tracking excited state decay mechanisms of pyrimidine nucleosides in real time.. <i>Nature Communications</i> , 2021 , 12, 7285	17.4	3
16	Soft X-ray Spectroscopic Properties of Ruthenium Complex Catalyst under CO ₂ Electrochemical Reduction Conditions: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 22899-22907	3.8	2
15	Ternary Complex Formation and Photoactivation of a Photoenzyme Results in Altered Protein Dynamics. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 7372-7384	3.4	2
14	Boosting the Guerbet Reaction: a cooperative catalytic system for the efficient bio-ethanol refinery to second-generation biofuels. <i>Journal of Catalysis</i> , 2021 ,	7.3	2
13	Polymerization Isomerism in Co-M (M = Cu, Ag, Au) Carbonyl Clusters: Synthesis, Structures and Computational Investigation. <i>Molecules</i> , 2021 , 26,	4.8	2
12	Bimetallic CoM (M = Cu, Ag, and Au) Carbonyl Complexes Supported by N-Heterocyclic Carbene Ligands: Synthesis, Structures, Computational Investigation, and Catalysis for Ammonia Borane Dehydrogenation. <i>Organometallics</i> , 2021 , 40, 2724-2735	3.8	2
11	On the origin of controlled anisotropic growth of monodisperse gold nanobipyramids. <i>Nanoscale</i> , 2021 , 13, 15292-15300	7.7	2
10	Heterometallic rhodium clusters as electron reservoirs: Chemical, electrochemical, and theoretical studies of the centered-icosahedral [RhE(CO)] atomically precise carbonyl compounds. <i>Journal of Chemical Physics</i> , 2021 , 155, 104301	3.9	2
9	Ultrafast Carotenoid to Retinal Energy Transfer in Xanthorhodopsin Revealed by the Combination of Transient Absorption and Two-Dimensional Electronic Spectroscopy. <i>Chemistry - A European Journal</i> , 2018 , 24, 12084-12092	4.8	1
8	Computational Studies of the Oxygen-Evolving Complex of Photosystem II and Biomimetic Oxomanganese Complexes for Renewable Energy Applications. <i>ACS Symposium Series</i> , 2013 , 203-215	0.4	1
7	Distinct Allosteric Pathways in Imidazole Glycerol Phosphate Synthase from Yeast and Bacteria. <i>Biophysical Journal</i> , 2021 ,	2.9	1
6	Control of Protonated Schiff Base Excited State Decay within Visual Protein Mimics: A Unified Model for Retinal Chromophores. <i>Chemistry - A European Journal</i> , 2021 , 27, 16389-16400	4.8	1
5	Photo-Active Biological Molecular Materials: From Photoinduced Dynamics to Transient Electronic Spectroscopies. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2021 , 77-142	0.7	0
4	Structural Studies of Oxomanganese Complexes for Water Oxidation Catalysis 2014 , 1-14		
3	Two State Reactivity Paradigm in Catalysis. The Example of X?H (X = O, N, C) and C?C Bonds Activation Mediated by Transition Metal Compounds337-366		
2	Elucidating the Activation Mechanism of AMPK by Direct Pan-Activator PF-739. <i>Frontiers in Molecular Biosciences</i> , 2021 , 8, 760026	5.6	
1	Two-State Reaction Paradigm in Transition Metals Mediated Reactions 2019 , 1115-1118		

