Ivan Rivalta

List of Publications by Year in Descending Order

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	Elucidating the Activation Mechanism of AMPK by Direct Pan-Activator PF-739. *Frontiers in Molecular Biosciences*, **2021**, 8, 760026	5.6	
88	Photo-Active Biological Molecular Materials: From Photoinduced Dynamics to Transient Electronic Spectroscopies. *Challenges and Advances in Computational Chemistry and Physics*, **2021**, 77-142	0.7	0
87	Boosting the Guerbet Reaction: a cooperative catalytic system for the efficient bio-ethanol refinery to second-generation biofuels. *Journal of Catalysis*, **2021**,	7.3	2
86	Distinct Allosteric Pathways in Imidazole Glycerol Phosphate Synthase from Yeast and Bacteria. *Biophysical Journal*, **2021**,	2.9	1
85	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	4.8	1
84	Polymerization Isomerism in Co-M (M = Cu, Ag, Au) Carbonyl Clusters: Synthesis, Structures and Computational Investigation. *Molecules*, **2021**, 26,	4.8	2
83	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. *Organometallics*, **2021**, 40, 2724-2735	3.8	2
82	On the origin of controlled anisotropic growth of monodisperse gold nanobipyramids. *Nanoscale*, **2021**, 13, 15292-15300	7.7	2
81	Heterometallic rhodium clusters as electron reservoirs: Chemical, electrochemical, and theoretical studies of the centered-icosahedral [RhE(CO)] atomically precise carbonyl compounds. *Journal of Chemical Physics*, **2021**, 155, 104301	3.9	2
80	Community Network Analysis of Allosteric Proteins. *Methods in Molecular Biology*, **2021**, 2253, 137-151	1.4	8
79	Tracking excited state decay mechanisms of pyrimidine nucleosides in real time.. *Nature Communications*, **2021**, 12, 7285	17.4	3
78	Detecting Dissociation Dynamics of Phosphorus Molecular Ions by Atom Probe Tomography. *Journal of Physical Chemistry A*, **2020**, 124, 10977-10988	2.8	4
77	Simulating Plasmon Resonances of Gold Nanoparticles with Bipyramidal Shapes by Boundary Element Methods. *Journal of Chemical Theory and Computation*, **2020**, 16, 3807-3815	6.4	9
76	First-principles characterization of the singlet excited state manifold in DNA/RNA nucleobases. *Physical Chemistry Chemical Physics*, **2020**, 22, 15496-15508	3.6	6
75	Decrypting the Information Exchange Pathways across the Spliceosome Machinery. *Journal of the American Chemical Society*, **2020**, 142, 8403-8411	16.4	13
74	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	3.6	3
73	Exploring Allosteric Pathways of a V-Type Enzyme with Dynamical Perturbation Networks. *Journal of Physical Chemistry B*, **2019**, 123, 3452-3461	3.4	14

72	Allostery in Its Many Disguises: From Theory to Applications. *Structure*, **2019**, 27, 566-578	5.2	158
71	Ternary Complex Formation and Photoactivation of a Photoenzyme Results in Altered Protein Dynamics. *Journal of Physical Chemistry B*, **2019**, 123, 7372-7384	3.4	2
70	Two-State Reaction Paradigm in Transition Metals Mediated Reactions **2019**, 1115-1118		
69	Two-dimensional UV spectroscopy: a new insight into the structure and dynamics of biomolecules. *Chemical Science*, **2019**, 10, 9907-9921	9.4	24
68	Towards Accurate Simulation of Two-Dimensional Electronic Spectroscopy. *Topics in Current Chemistry Collections*, **2019**, 63-112	1.8	3
67	Modeling multidimensional spectral lineshapes from first principles: application to water-solvated adenine. *Faraday Discussions*, **2019**, 221, 219-244	3.6	17
66	The highly excited-state manifold of guanine: calibration for nonlinear electronic spectroscopy simulations. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	10
65	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	6.4	12
64	UV-induced long-lived decays in solvated pyrimidine nucleosides resolved at the MS-CASPT2/MM level. *Physical Chemistry Chemical Physics*, **2018**, 20, 6877-6890	3.6	32
63	The effect of solvent relaxation in the ultrafast time-resolved spectroscopy of solvated benzophenone. *Photochemical and Photobiological Sciences*, **2018**, 17, 323-331	4.2	8
62	Two-dimensional electronic spectroscopy as a tool for tracking molecular conformations in DNA/RNA aggregates. *Faraday Discussions*, **2018**, 207, 233-250	3.6	10
61	Ultrafast Carotenoid to Retinal Energy Transfer in Xanthorhodopsin Revealed by the Combination of Transient Absorption and Two-Dimensional Electronic Spectroscopy. *Chemistry - A European Journal*, **2018**, 24, 12084-12092	4.8	1
60	Theoretical Model of the Protochlorophyllide Oxidoreductase from a Hierarchy of Protocols. *Journal of Physical Chemistry B*, **2018**, 122, 7668-7681	3.4	7
59	Towards Accurate Simulation of Two-Dimensional Electronic Spectroscopy. *Topics in Current Chemistry*, **2018**, 376, 24	7.2	16
58	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	11.5	72
57	Key role of the REC lobe during CRISPR-Cas9 activation by 'sensing', 'regulating', and 'locking' the catalytic HNH domain. *Quarterly Reviews of Biophysics*, **2018**, 51,	7	42
56	COBRAMM 2.0 - A software interface for tailoring molecular electronic structure calculations and running nanoscale (QM/MM) simulations. *Journal of Molecular Modeling*, **2018**, 24, 271	2	29
55	Characterization of Protein Tyrosine Phosphatase 1B Inhibition by Chlorogenic Acid and Cichoric Acid. *Biochemistry*, **2017**, 56, 96-106	3.2	14

54	Fine Tuning of Retinal Photoinduced Decay in Solution. *Journal of Physical Chemistry Letters*, **2017**, 8, 4407-4412	6.4	14
53	Protospacer Adjacent Motif-Induced Allostery Activates CRISPR-Cas9. *Journal of the American Chemical Society*, **2017**, 139, 16028-16031	16.4	66
52	Allosteric Communication Disrupted by a Small Molecule Binding to the Imidazole Glycerol Phosphate Synthase Protein-Protein Interface. *Biochemistry*, **2016**, 55, 6484-6494	3.2	25
51	Multiple Decay Mechanisms and 2D-UV Spectroscopic Fingerprints of Singlet Excited Solvated Adenine-Uracil Monophosphate. *Chemistry - A European Journal*, **2016**, 22, 7497-507	4.8	26
50	Dissecting Dynamic Allosteric Pathways Using Chemically Related Small-Molecule Activators. *Structure*, **2016**, 24, 1155-66	5.2	29
49	Allosteric Pathways in the PPAR□RXR□nuclear receptor complex. *Scientific Reports*, **2016**, 6, 19940	4.9	31
48	Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. *Journal of Computational Chemistry*, **2016**, 37, 506-41	3.5	1047
47	Ultraviolet vision: photophysical properties of the unprotonated retinyl Schiff base in the Siberian hamster cone pigment. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	4
46	Spectroscopic fingerprints of DNA/RNA pyrimidine nucleobases in third-order nonlinear electronic spectra. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	24
45	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, 7291-302	3.6	31
44	Tracking the primary photoconversion events in rhodopsins by ultrafast optical spectroscopy. *Photochemical and Photobiological Sciences*, **2015**, 14, 213-28	4.2	27
43	Triplet Oxygen Evolution Catalyzed by a Biomimetic Oxomanganese Complex: Functional Role of the Carboxylate Buffer. *ACS Catalysis*, **2015**, 5, 2384-2390	13.1	14
42	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	3.8	2
41	Two-Dimensional Electronic Spectroscopy of Benzene, Phenol, and Their Dimer: An Efficient First-Principles Simulation Protocol. *Journal of Chemical Theory and Computation*, **2015**, 11, 3755-71	6.4	23
40	Probing deactivation pathways of DNA nucleobases by two-dimensional electronic spectroscopy: first principles simulations. *Faraday Discussions*, **2015**, 177, 345-62	3.6	27
39	Modeling the high-energy electronic state manifold of adenine: Calibration for nonlinear electronic spectroscopy. *Journal of Chemical Physics*, **2015**, 142, 212443	3.9	37
38	Deciphering the photochemical mechanisms describing the UV-induced processes occurring in solvated guanine monophosphate. *Frontiers in Chemistry*, **2015**, 3, 29	5	23
37	Spectral lineshapes in nonlinear electronic spectroscopy. *Physical Chemistry Chemical Physics*, **2015**, 17, 30925-36	3.6	34

36	Facile Ecofriendly Synthesis of Monastrol and Its Structural Isomers via Biginelli Reaction. *ACS Sustainable Chemistry and Engineering*, **2014**, 2, 1228-1233	8.3	44
35	Modelling retinal chromophores photoisomerization: from minimal models in vacuo to ultimate bidimensional spectroscopy in rhodopsins. *Physical Chemistry Chemical Physics*, **2014**, 16, 16865-79	3.6	30
34	Modelling time-resolved two-dimensional electronic spectroscopy of the primary photoisomerization event in rhodopsin. *Journal of Physical Chemistry B*, **2014**, 118, 8396-405	3.4	27
33	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	6.4	31
32	Structural Studies of Oxomanganese Complexes for Water Oxidation Catalysis **2014**, 1-14		
31	Tracking conformational dynamics of polypeptides by nonlinear electronic spectroscopy of aromatic residues: a first-principles simulation study. *ChemPhysChem*, **2014**, 15, 3282-90	3.2	22
30	Bidimensional electronic spectroscopy on indole in gas phase and in water from first principles. *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 295-303	2	20
29	Ab initio simulations of two-dimensional electronic spectra: The SOS//QM/MM approach. *International Journal of Quantum Chemistry*, **2014**, 114, 85-93	2.1	34
28	Characterization of an amorphous iridium water-oxidation catalyst electrodeposited from organometallic precursors. *Inorganic Chemistry*, **2013**, 52, 1860-71	5.1	59
27	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, 6217-26	3.4	32
26	Computational Studies of the Oxygen-Evolving Complex of Photosystem II and Biomimetic Oxomanganese Complexes for Renewable Energy Applications. *ACS Symposium Series*, **2013**, 203-215	0.4	1
25	Solution NMR and computational methods for understanding protein allostery. *Journal of Physical Chemistry B*, **2013**, 117, 3063-73	3.4	35
24	Spectral tuning of ultraviolet cone pigments: an interhelical lock mechanism. *Journal of the American Chemical Society*, **2013**, 135, 19064-7	16.4	20
23	Allosteric pathways in imidazole glycerol phosphate synthase. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, E1428-36	11.5	142
22	Oxomanganese complexes for natural and artificial photosynthesis. *Current Opinion in Chemical Biology*, **2012**, 16, 11-8	9.7	73
21	Reengineering rate-limiting, millisecond enzyme motions by introduction of an unnatural amino acid. *Biophysical Journal*, **2011**, 101, 411-20	2.9	13
20	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	6.4	28
19	S1-state model of the O2-evolving complex of photosystem II. *Biochemistry*, **2011**, 50, 6308-11	3.2	196

18	Structural-functional role of chloride in photosystem II. *Biochemistry*, **2011**, 50, 6312-5	3.2	114
17	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	2.5	5
16	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	2.5	20
15	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, 1350-60	6.4	23
14	The geometric effect in palladium-gold catalysis. Is the coupling the rate-determining step in the vinyl-acetate synthesis?. *Chemical Communications*, **2009**, 1852-4	5.8	14
13	Interaction of CO with PdAu(111) and PdAu(100) Bimetallic Surfaces: A Theoretical Cluster Model Study. *Journal of Physical Chemistry C*, **2008**, 112, 6073-6081	3.8	35
12	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, 1283-92	6.4	21
11	Theoretical study of the gas-phase ethane C□H and C□C bonds activation by bare niobium cation. *Theoretical Chemistry Accounts*, **2008**, 120, 395-403	1.9	8
10	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	2.5	15
9	Pd, Rh, Ir and Pt adsorption on gold: A theoretical study of different surfaces. *Chemical Physics Letters*, **2007**, 442, 105-109	2.5	5
8	On the insertion mechanism of molecular oxygen into a Pd(II)□H bond. Something to add. *Chemical Physics Letters*, **2007**, 443, 183-189	2.5	24
7	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	1.9	36
6	Methane activation by chromium oxide cations in the gas phase: a theoretical study. *Journal of Computational Chemistry*, **2006**, 27, 174-87	3.5	30
5	Activation of methane by the iron dimer cation. A theoretical study. *Journal of Physical Chemistry A*, **2006**, 110, 12501-11	2.8	23
4	A theoretical study of ethylene dehydrogenation by bare Niobium atom and cation. *Computational and Theoretical Chemistry*, **2006**, 762, 25-31		14
3	Acetylene cyclotrimerization by early second-row transition metals in the gas phase. A theoretical study. *Inorganic Chemistry*, **2005**, 44, 9807-16	5.1	26
2	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		
1	Tracking excited state decay mechanisms of pyrimidine nucleosides in real time		3