Maurizio Bruschi

List of Publications by Citations

87 papers	2,791 citations	30 h-index	50 g-index
89 ext. papers	2,995 ext. citations	6.8 avg, IF	4.69 L-index

#	Paper	IF	Citations
87	Synthesis of the H-cluster framework of iron-only hydrogenase. *Nature*, **2005**, 433, 610-3	50.4	467
86	A QM/MM investigation of the activation and catalytic mechanism of Fe-only hydrogenases. *Inorganic Chemistry*, **2007**, 46, 5911-21	5.1	109
85	Molecular determinants of the physicochemical properties of a critical prion protein region comprising residues 106126. *Biochemical Journal*, **1999**, 342, 207-214	3.8	94
84	Investigations on the role of proton-coupled electron transfer in hydrogen activation by [FeFe]-hydrogenase. *Journal of the American Chemical Society*, **2014**, 136, 15394-402	16.4	86
83	DFT investigation of structural, electronic, and catalytic properties of diiron complexes related to the [2Fe](H) subcluster of Fe-only hydrogenases. *Inorganic Chemistry*, **2002**, 41, 1421-9	5.1	82
82	Influence of the [2Fe]H subcluster environment on the properties of key intermediates in the catalytic cycle of [FeFe] hydrogenases: hints for the rational design of synthetic catalysts. *Angewandte Chemie - International Edition*, **2009**, 48, 3503-6	16.4	79
81	Gas-phase reaction of phenol with NO3. *Environmental Science & Technology*, **2001**, 35, 1791-7	10.3	79
80	Insights into the mechanism of electrocatalytic hydrogen evolution mediated by Fe2(S2C3H6)(CO)6: the simplest functional model of the Fe-hydrogenase active site. *Inorganic Chemistry*, **2007**, 46, 108-16	5.1	77
79	The oxidative inactivation of FeFe hydrogenase reveals the flexibility of the H-cluster. *Nature Chemistry*, **2014**, 6, 336-42	17.6	75
78	Density functional theory investigation of the active site of [Fe]-hydrogenases: effects of redox state and ligand characteristics on structural, electronic, and reactivity properties of complexes related to the [2Fe]H subcluster. *Inorganic Chemistry*, **2003**, 42, 4773-81	5.1	75
77	Synthesis, Electronic Characterisation and Significant Second-Order Non-Linear Optical Responses of meso-Tetraphenylporphyrins and Their ZnII Complexes Carrying a Push or Pull Group in the Pyrrolic Position. *European Journal of Inorganic Chemistry*, **2005**, 2005, 3857-3874	2.3	58
76	Disclosure of key stereoelectronic factors for efficient H2 binding and cleavage in the active site of [NiFe]-hydrogenases. *Journal of the American Chemical Society*, **2014**, 136, 1803-14	16.4	57
75	Density functional theory investigation of the active site of Fe-hydrogenases. systematic study of the effects of redox state and ligands hardness on structural and electronic properties of complexes related to the [2Fe](H) subcluster. *Inorganic Chemistry*, **2004**, 43, 3733-41	5.1	56
74	Theoretical Study of Hydration of Cyanamide and Carbodiimide. *Journal of Physical Chemistry A*, **2003**, 107, 1188-1196	2.8	56
73	Structural and electronic properties of the [FeFe] hydrogenase H-cluster in different redox and protonation states. A DFT investigation. *Inorganic Chemistry*, **2008**, 47, 6056-71	5.1	54
72	Catalytic Mechanism of Fungal Lytic Polysaccharide Monooxygenases Investigated by First-Principles Calculations. *Inorganic Chemistry*, **2018**, 57, 86-97	5.1	54
71	Nucleolin, a novel partner for the Myb transcription factor family that regulates their activity. *Journal of Biological Chemistry*, **2000**, 275, 4152-8	5.4	50

70	Targeting intermediates of [FeFe]-hydrogenase by CO and CN vibrational signatures. *Inorganic Chemistry*, **2011**, 50, 3888-900	5.1	48
69	A theoretical study of spin states in Ni-S4 complexes and models of the [NiFe] hydrogenase active site. *Journal of Biological Inorganic Chemistry*, **2004**, 9, 873-84	3.7	47
68	Dissecting the intimate mechanism of cyanation of {2Fe3S} complexes related to the active site of all-iron hydrogenases by DFT analysis of energetics, transition states, intermediates and products in the carbonyl substitution pathway. *Chemistry - A European Journal*, **2005**, 11, 509-20	4.8	43
67	Structural insights into the active-ready form of [FeFe]-hydrogenase and mechanistic details of its inhibition by carbon monoxide. *Inorganic Chemistry*, **2007**, 46, 7256-8	5.1	42
66	Electronic Characterisation and Significant Second-Order NLO Response of 10,20-Diphenylporphyrins and Their ZnII Complexes Substituted in the meso Position with Delocalised Linkers Carrying Push or Pull Groups. *European Journal of Inorganic Chemistry*, **2006**, 2006, 1743-1757	2.3	41
65	Nitrosyl derivatives of diiron(I) dithiolates mimic the structure and Lewis acidity of the [FeFe]-hydrogenase active site. *Journal of the American Chemical Society*, **2008**, 130, 12021-30	16.4	40
64	Uncovering a dynamically formed substrate access tunnel in carbon monoxide dehydrogenase/acetyl-CoA synthase. *Journal of the American Chemical Society*, **2013**, 135, 9493-502	16.4	38
63	trans versus geminal electron delocalization in tetra- and diethynylethenes: a new method of analysis. *Chemistry - A European Journal*, **2002**, 8, 4216-27	4.8	37
62	Mechanistic and physiological implications of the interplay among iron-sulfur clusters in [FeFe]-hydrogenases. A QM/MM perspective. *Journal of the American Chemical Society*, **2011**, 133, 18742-9	16.4	36
61	Combining experimental and theoretical methods to learn about the reactivity of gas-processing metalloenzymes. *Energy and Environmental Science*, **2014**, 7, 3543-3573	35.4	33
60	Molecular determinants of the physicochemical properties of a critical prion protein region comprising residues 106-126. *Biochemical Journal*, **1999**, 342, 207	3.8	33
59	Functionally relevant interplay between the Fe(4)S(4) cluster and CN(-) ligands in the active site of [FeFe]-hydrogenases. *Journal of the American Chemical Society*, **2010**, 132, 4992-3	16.4	31
58	Electron delocalization in linearly pi-conjugated systems: a concept for quantitative analysis. *Chemistry - A European Journal*, **2004**, 10, 5671-80	4.8	30
57	DFT Investigation of H2 activation by [M(NHPnPr3)(S3O)] (M = Ni, Pd). Insight into key factors relevant to the design of hydrogenase functional models. *Journal of the American Chemical Society*, **2005**, 127, 13180-9	16.4	29
56	CO Affinity and Bonding Properties of [FeFe] Hydrogenase Active Site Models. A DFT Study. *Organometallics*, **2010**, 29, 2013-2025	3.8	27
55	Electrocatalytic dihydrogen evolution mechanism of [Fe2(CO)4(kappa(2)-Ph2PCH2CH2PPh2)(mu-S(CH2)3S)] and related models of the [FeFe]-hydrogenases active site: a DFT investigation. *Dalton Transactions*, **2010**, 39, 7320-9	4.3	26
54	Online Quantification of Criegee Intermediates of Pinene Ozonolysis by Stabilization with Spin Traps and Proton-Transfer Reaction Mass Spectrometry Detection. *Journal of the American Chemical Society*, **2017**, 139, 3999-4008	16.4	25
53	A Scheme for the Evaluation of Electron Delocalization and Conjugation Efficiency in Linearly Conjugated Systems. *Journal of Chemical Theory and Computation*, **2009**, 5, 506-14	6.4	25

52	Isolation and characterization of the gene coding for human cytidine deaminase. *Biochimica Et Biophysica Acta Gene Regulatory Mechanisms*, **1998**, 1443, 323-33		25
51	A DFT study of EPR parameters in Cu(II) complexes of the octarepeat region of the prion protein. *Physical Chemistry Chemical Physics*, **2008**, 10, 4573-83	3.6	24
50	Tailoring transition metal complexes for nonlinear optics applications. 2. A theoretical investigation of the second-order nonlinear optical properties of M(CO)(5)L complexes (M = Cr, W; L = Py, PyCHO, Pyz, PyzBF(3), BPE, BPEBF(3)). *Journal of Physical Chemistry A*, **2005**, 109, 9637-45	2.8	24
49	Redox non-innocence of a N-heterocyclic nitrenium cation bound to a nickel-cyclam core. *Journal of the American Chemical Society*, **2014**, 136, 582-5	16.4	23
48	Impact of Cadmium on Intracellular Zinc Levels in HepG2 Cells: Quantitative Evaluations and Molecular Effects. *BioMed Research International*, **2015**, 2015, 949514	3	21
47	Magnetic Properties of [FeFe]-Hydrogenases: A Theoretical Investigation Based on Extended QM and QM/MM Models of the H-Cluster and Its Surroundings. *European Journal of Inorganic Chemistry*, **2011**, 2011, 1043-1049	2.3	20
46	Asymmetric biomimetic oxidations of phenols using oxazolidines as chiral auxiliaries: the enantioselective synthesis of (+)- and (−)-dehydrodiconiferyl alcohol. *Journal of Physical Organic Chemistry*, **2006**, 19, 592-596	2.1	20
45	A multitechnique investigation of the second order NLO response of a 10,20-diphenylporphyrinato nickel(II) complex carrying a phenylethynyl based push-pull system in the 5- and 15-positions. *Journal of Porphyrins and Phthalocyanines*, **2004**, 08, 1311-1324	1.8	19
44	Isocyanide in biochemistry? A theoretical investigation of the electronic effects and energetics of cyanide ligand protonation in [FeFe]-hydrogenases. *Chemistry - A European Journal*, **2011**, 17, 1954-65	4.8	16
43	Through versus cross electron delocalization in polytriacetylene oligomers: a computational analysis. *ChemPhysChem*, **2005**, 6, 511-9	3.2	16
42	Structure and energetics of Fe2(CO)8 singlet and triplet electronic states. *Journal of Physical Chemistry A*, **2007**, 111, 12152-62	2.8	15
41	Influence of a Large π-Donor Ligand on Structural and Catalytic Properties of Di-Iron Compounds Related to the Active Site of Fe-Hydrogenase—A DFT Investigation. *European Journal of Inorganic Chemistry*, **2007**, 2007, 1835-1843	2.3	15
40	Interaction of the H-Cluster of FeFe Hydrogenase with Halides. *Journal of the American Chemical Society*, **2018**, 140, 5485-5492	16.4	14
39	Reaction products and mechanism of the regioselective oxidation of N-phenylmorpholine by ozone. *Tetrahedron*, **2012**, 68, 8267-8275	2.4	14
38	Photoinhibition of FeFe Hydrogenase. *ACS Catalysis*, **2017**, 7, 7378-7387	13.1	13
37	A DFT investigation on structural and redox properties of a synthetic Fe6S6 assembly closely related to the [FeFe]-hydrogenases active site. *Comptes Rendus Chimie*, **2008**, 11, 834-841	2.7	13
36	Reactivation of the Ready and Unready Oxidized States of [NiFe]-Hydrogenases: Mechanistic Insights from DFT Calculations. *Inorganic Chemistry*, **2019**, 58, 279-293	5.1	13
35	Asymmetric biomimetic oxidations of phenols: the mechanism of the diastereo- and enantioselective synthesis of thomasidioic acid. *Molecules*, **2008**, 13, 129-48	4.8	12

34	H Activation in [FeFe]-Hydrogenase Cofactor Versus Diiron Dithiolate Models: Factors Underlying the Catalytic Success of Nature and Implications for an Improved Biomimicry. *Chemistry - A European Journal*, **2019**, 25, 1227-1241	4.8	12
33	Metal(loid)s role in the pathogenesis of amyotrophic lateral sclerosis: Environmental, epidemiological, and genetic data. *Environmental Research*, **2021**, 192, 110292	7.9	12
32	Does the environment around the H-cluster allow coordination of the pendant amine to the catalytic iron center in [FeFe]□hydrogenases? Answers from theory. *Journal of Biological Inorganic Chemistry*, **2013**, 18, 693-700	3.7	11
31	A new multivalent cluster: synthesis, electrochemistry, solid state structure and computational studies on the iron□nickel mixed-metal nitride anions [Fe6Ni6N2(CO)24]n□(n=2□). *Comptes Rendus Chimie*, **2005**, 8, 1850-1855	2.7	11
30	Theoretical investigation of aerobic and anaerobic oxidative inactivation of the [NiFe]-hydrogenase active site. *Physical Chemistry Chemical Physics*, **2018**, 20, 1693-1706	3.6	10
29	Towards biomimetic models of the reduced [FeFe]-hydrogenase that preserve the key structural features of the enzyme active site; a DFT investigation. *International Journal of Hydrogen Energy*, **2014**, 39, 18565-18573	6.7	10
28	Tetrameric Silver(I) Complex with Bridging N-Heterocyclic Carbene Ligands: [(iPrIm)Ag(NO3)]4. *Organometallics*, **2014**, 33, 5610-5613	3.8	10
27	Probing the effects of one-electron reduction and protonation on the electronic properties of the Fe-S clusters in the active-ready form of [FeFe]-hydrogenases. A QM/MM investigation. *ChemPhysChem*, **2011**, 12, 3376-82	3.2	10
26	Structural variations, electrochemical properties and computational studies on monomeric and dimeric Fe-Cu carbide clusters, forming copper-based staple arrays. *Dalton Transactions*, **2011**, 40, 5464-75	4.3	10
25	Distinct Lipid Transfer Proteins display different IgE-binding activities that are affected by fatty acid binding. *Allergy: European Journal of Allergy and Clinical Immunology*, **2019**, 74, 827-831	9.3	10
24	A new FeMo complex as a model of heterobimetallic assemblies in natural systems: M□ssbauer and density functional theory investigations. *Inorganic Chemistry*, **2014**, 53, 11345-7	5.1	9
23	Theoretical insights into [NiFe]-hydrogenases oxidation resulting in a slowly reactivating inactive state. *Journal of Biological Inorganic Chemistry*, **2017**, 22, 137-151	3.7	9
22	Speciation of copper-peptide complexes in water solution using DFTB and DFT approaches: case of the [Cu(HGGG)(Py)] complex. *Journal of Physical Chemistry B*, **2012**, 116, 6250-60	3.4	9
21	Tailoring transition metal complexes for non linear optics applications: A theoretical investigation of the electronic structure of M(CO)xClyL complexes (M = Cr, W, Re, Ru, Os, Rh, Ir; L = Pyz, PyzBF3, BPE, BPEBF3). *Journal of Molecular Catalysis A*, **2003**, 204-205, 793-803		9
20	Computational approaches to the prediction of the redox potentials of iron and copper bioinorganic systems. *International Journal of Quantum Chemistry*, **2016**, 116, 1695-1705	2.1	9
19	Copper coordination to the putative cell binding site of angiogenin: a DFT investigation. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	8
18	Computational approaches to shed light on molecular mechanisms in biological processes. *Theoretical Chemistry Accounts*, **2007**, 117, 723-741	1.9	8
17	First-Principles Calculations on Ni,Fe-Containing Carbon Monoxide Dehydrogenases Reveal Key Stereoelectronic Features for Binding and Release of CO to/from the C-Cluster. *Inorganic Chemistry* , **2021**, 60, 387-402	5.1	8

16	Influence of the [2Fe]H Subcluster Environment on the Properties of Key Intermediates in the Catalytic Cycle of [FeFe] Hydrogenases: Hints for the Rational Design of Synthetic Catalysts. *Angewandte Chemie*, **2009**, 121, 3555-3558	3.6	7
15	Quantum Chemical Investigations of Reaction Paths of Metalloenzymes and Biomimetic Models The Hydrogenase Example. *Topics in Current Chemistry*, **2006**, 1-46		7
14	N-aryl lactams by regioselective ozonation of N-aryl cyclic amines. *ISRN Organic Chemistry*, **2012**, 2012, 281642		6
13	Relation between coordination geometry and stereoelectronic properties in DFT models of the CO-inhibited [FeFe]-hydrogenase cofactor. *Journal of Organometallic Chemistry*, **2009**, 694, 2846-2853	2.3	5
12	The regiochemistry of the NO3-promoted gas phase nitration of toluene and phenol with NO2. *Journal of Physical Organic Chemistry*, **2006**, 19, 570-578	2.1	5
11	Measuring Electron Delocalization in Conjugated Systems. *Chimia*, **2005**, 59, 539-544	1.3	5
10	FeMo Heterobimetallic Dithiolate Complexes: Investigation of Their Electron Transfer Chemistry and Reactivity toward Acids, a Density Functional Theory Rationalization. *Inorganic Chemistry*, **2019**, 58, 679-694	5.1	5
9	Influence of key amino acid mutation on the active site structure and on folding in acetyl-CoA synthase: a theoretical perspective. *Chemical Communications*, **2015**, 51, 8551-4	5.8	4
8	Redox Potentials of Small Inorganic Radicals and Hexa-Aquo Complexes of First-Row Transition Metals in Water: A DFT Study Based on the Grand Canonical Ensemble. *Journal of Physical Chemistry A*, **2019**, 123, 6948-6957	2.8	4
7	Copper ion interaction with the RNase catalytic site fragment of the angiogenin protein: an experimental and theoretical investigation. *Dalton Transactions*, **2017**, 46, 8524-8538	4.3	3
6	The Challenging Description of Carbon Monoxide Oxidation as Catalyzed by Molybdenum-Copper CO Dehydrogenase. *Frontiers in Chemistry*, **2018**, 6, 630	5	3
5	Quantum mechanical methods for the investigation of metalloproteins and related bioinorganic compounds. *Methods in Molecular Biology*, **2014**, 1122, 207-68	1.4	2
4	Podophyllotoxin and Antitumor Synthetic Aryltetralines. Toward a Biomimetic Preparation **2010**,		1
3	Hydrogenases: Theoretical Investigations Towards Bioinspired H2 Production and Activation **2009**,		1
2	Theoretical Insights into the Aerobic Hydrogenase Activity of Molybdenum Copper CO Dehydrogenase. *Inorganics*, **2019**, 7, 135	2.9	1
1	Copper coordination to the putative cell binding site of angiogenin: a DFT investigation. *Highlights in Theoretical Chemistry*, **2013**, 255-269		0