Maurizio Bruschi

List of Publications by Year
in descending order

85 papers	3,127 citations	159358 30 h-index	168136 53 g-index
89 all docs	89 docs citations	89 times ranked	2933 citing authors

#	Article	IF	Citations
1	Synthesis of the H-cluster framework of iron-only hydrogenase. Nature, 2005, 433, 610-613.	13.7	498
2	A QM/MM Investigation of the Activation and Catalytic Mechanism of Fe-Only Hydrogenases. Inorganic Chemistry, 2007, 46, 5911-5921.	1.9	112
3	Investigations on the Role of Proton-Coupled Electron Transfer in Hydrogen Activation by [FeFe]-Hydrogenase. Journal of the American Chemical Society, 2014, 136, 15394-15402.	6.6	107
4	Molecular determinants of the physicochemical properties of a critical prion protein region comprising residues 106â€“126. Biochemical Journal, 1999, 342, 207-214.	1.7	100
5	Gas-Phase Reaction of Phenol with NO3. Environmental Science & Technology, 2001, 35, 1791-1797.	4.6	94
6	DFT Investigation of Structural, Electronic, and Catalytic Properties of Diiron Complexes Related to the [2Fe]HSubcluster of Fe-Only Hydrogenases. Inorganic Chemistry, 2002, 41, 1421-1429.	1.9	86
7	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, 3503-3506.	7.2	86
8	Insights into the Mechanism of Electrocatalytic Hydrogen Evolution Mediated by Fe2(S2C3H6)(CO)6:Â The Simplest Functional Model of the Fe-Hydrogenase Active Site. Inorganic Chemistry, 2007, 46, 108-116.	1.9	85
9	The oxidative inactivation of FeFe hydrogenase reveals the flexibility of the H-cluster. Nature Chemistry, 2014, 6, 336-342.	6.6	83
10	Density Functional Theory Investigation of the Active Site of [Fe]-Hydrogenases:â€‰ 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, 4773-4781.	1.9	78
11	Catalytic Mechanism of Fungal Lytic Polysaccharide Monooxygenases Investigated by First-Principles Calculations. Inorganic Chemistry, 2018, 57, 86-97.	1.9	72
12	Synthesis, Electronic Characterisation and Significant Second-Order Non-Linear Optical Responses ofmeso-Tetraphenylporphyrins and Their ZnII Complexes Carrying a Push or Pull Group in the Î² Pyrrolic Position. European Journal of Inorganic Chemistry, 2005, 2005, 3857-3874.	1.0	68
13	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, 1803-1814.	6.6	68
14	Theoretical Study of Hydration of Cyanamide and Carbodiimide. Journal of Physical Chemistry A, 2003, 107, 1188-1196.	1.1	62
15	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, 3733-3741.	1.9	60
16	Structural and Electronic Properties of the [FeFe] Hydrogenase H-Cluster in Different Redox and Protonation States. A DFT Investigation. Inorganic Chemistry, 2008, 47, 6056-6071.	1.9	58
17	Nucleolin, a Novel Partner for the Myb Transcription Factor Family That Regulates Their Activity. Journal of Biological Chemistry, 2000, 275, 4152-4158.	1.6	54
18	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, 873-884.	1.1	52

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19	Targeting Intermediates of [FeFe]-Hydrogenase by CO and CN Vibrational Signatures. Inorganic Chemistry, 2011, 50, 3888-3900.	1.9	51
20	Electronic Characterisation and Significant Second-Order NLO Response of 10,20-Diphenylporphyrins and Their ZnII Complexes Substituted in themeso Position with Ï€-Delocalised Linkers Carrying Push or Pull Groups. European Journal of Inorganic Chemistry, 2006, 2006, 1743-1757.	1.0	48
21	Uncovering a Dynamically Formed Substrate Access Tunnel in Carbon Monoxide Dehydrogenase/Acetyl-CoA Synthase. Journal of the American Chemical Society, 2013, 135, 9493-9502.	6.6	47
22	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, 509-533.	1.7	46
23	Structural Insights into the Active-Ready Form of [FeFe]-Hydrogenase and Mechanistic Details of Its Inhibition by Carbon Monoxide. Inorganic Chemistry, 2007, 46, 7256-7258.	1.9	44
24	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, 12021-12030.	6.6	44
25	trans versus geminal Electron Delocalization in Tetra- and Diethynylethenes: A New Method of Analysis. Chemistry - A European Journal, 2002, 8, 4216-4227.	1.7	40
26	Mechanistic and Physiological Implications of the Interplay among Ironâ€“Sulfur Clusters in [FeFe]-Hydrogenases. A QM/MM Perspective. Journal of the American Chemical Society, 2011, 133, 18742-18749.	6.6	38
27	Molecular determinants of the physicochemical properties of a critical prion protein region comprising residues 106â€’126. Biochemical Journal, 1999, 342, 207.	1.7	36
28	Combining experimental and theoretical methods to learn about the reactivity of gas-processing metalloenzymes. Energy and Environmental Science, 2014, 7, 3543-3573.	15.6	36
29	Functionally Relevant Interplay between the Fe₄S₄ Cluster and CN^{â^'} Ligands in the Active Site of [FeFe]-Hydrogenases. Journal of the American Chemical Society, 2010, 132, 4992-4993.	6.6	34
30	Electron Delocalization in Linearly Ï€-Conjugated Systems: A Concept for Quantitative Analysis. Chemistry - A European Journal, 2004, 10, 5671-5680.	1.7	33
31	DFT Investigation of H2Activation by [M(NHPnPr3)(â€˜S3â€˜)] (M = Ni, Pd). Insight into Key Factors Relevant to the Design of Hydrogenase Functional Models. Journal of the American Chemical Society, 2005, 127, 13180-13189.	6.6	31
32	Redox Non-Innocence of a N-Heterocyclic Nitrenium Cation Bound to a Nickelâ€“Cyclam Core. Journal of the American Chemical Society, 2014, 136, 582-585.	6.6	31
33	Isolation and characterization of the gene coding for human cytidine deaminase. Biochimica Et Biophysica Acta Gene Regulatory Mechanisms, 1998, 1443, 323-333.	2.4	30
34	Electrocatalytic dihydrogen evolution mechanism of [Fe2(CO)4(Îº2-Ph2PCH2CH2PPh2)(Î¼-S(CH2)3S)] and related models of the [FeFe]-hydrogenases active site: a DFT investigation. Dalton Transactions, 2010, 39, 7320.	1.6	29
35	Online Quantification of Criegee Intermediates of Î±-Pinene Ozonolysis by Stabilization with Spin Traps and Proton-Transfer Reaction Mass Spectrometry Detection. Journal of the American Chemical Society, 2017, 139, 3999-4008.	6.6	29
36	A Scheme for the Evaluation of Electron Delocalization and Conjugation Efficiency in Linearly Ï€-Conjugated Systems. Journal of Chemical Theory and Computation, 2009, 5, 506-514.	2.3	28

#	Article	IF	Citations
37	CO Affinity and Bonding Properties of [FeFe] Hydrogenase Active Site Models. A DFT Study. Organometallics, 2010, 29, 2013-2025.	1.1	28
38	Impact of Cadmium on Intracellular Zinc Levels in HepG2 Cells: Quantitative Evaluations and Molecular Effects. BioMed Research International, 2015, 2015, 1-10.	0.9	27
39	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.	1.3	26
40	Interaction of the H-Cluster of FeFe Hydrogenase with Halides. Journal of the American Chemical Society, 2018, 140, 5485-5492.	6.6	25
41	Tailoring Transition Metal Complexes for Nonlinear Optics Applications. 2. A Theoretical Investigation of the Second-Order Nonlinear Optical Properties of M(CO)5L Complexes (M = Cr, W; L = Py, PyCHO,) Tj ETQq1 1 0.784314 rgBT /Overl	1.7	23
42	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.	0.4	22
43	Asymmetric biomimetic oxidations of phenols using oxazolidines as chiral auxiliaries: the enantioselective synthesis of (+)- and (â^')-dehydrodiconiferyl alcohol. Journal of Physical Organic Chemistry, 2006, 19, 592-596.	0.9	21
44	Magnetic Properties of [FeFe]â€Hydrogenases: A Theoretical Investigation Based on Extended QM and QM/MM Models of the Hâ€Cluster and Its Surroundings. European Journal of Inorganic Chemistry, 2011, 2011, 1043-1049.	1.0	21
45	Photoinhibition of FeFe Hydrogenase. ACS Catalysis, 2017, 7, 7378-7387.	5.5	17
46	Distinct Lipid Transfer Proteins display different IgEâ€binding activities that are affected by fatty acid binding. Allergy: European Journal of Allergy and Clinical Immunology, 2019, 74, 827-831.	2.7	17
47	ThroughversusCrossElectron Delocalization in Polytriacetylene Oligomers: A Computational Analysis. ChemPhysChem, 2005, 6, 511-519.	1.0	16
48	Structure and Energetics of Fe2(CO)8Singlet and Triplet Electronic States. Journal of Physical Chemistry A, 2007, 111, 12152-12162.	1.1	16
49	Isocyanide in Biochemistry? A Theoretical Investigation of the Electronic Effects and Energetics of Cyanide Ligand Protonation in [FeFe]â€Hydrogenases. Chemistry - A European Journal, 2011, 17, 1954-1965.	1.7	16
50	Reaction products and mechanism of the regioselective oxidation of N-phenylmorpholine by ozone. Tetrahedron, 2012, 68, 8267-8275.	1.0	16
51	Computational approaches to the prediction of the redox potentials of iron and copper bioinorganic systems. International Journal of Quantum Chemistry, 2016, 116, 1695-1705.	1.0	16
52	H₂ Activation in [FeFe]â€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.	1.7	16
53	Metal(loid)s role in the pathogenesis of amyotrophic lateral sclerosis: Environmental, epidemiological, and genetic data. Environmental Research, 2021, 192, 110292.	3.7	16
54	Influence of a Large Ïƒ-Donor Ligand on Structural and Catalytic Properties of Di-Iron Compounds Related to the Active Site of Fe-Hydrogenase â€“ A DFT Investigation. European Journal of Inorganic Chemistry, 2007, 2007, 1835-1843.	1.0	15

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55	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.	3.8	15
56	First-Principles Calculations on Ni,Fe-Containing Carbon Monoxide Dehydrogenases Reveal Key Stereoelectronic Features for Binding and Release of CO₂ to/from the C-Cluster. Inorganic Chemistry, 2021, 60, 387-402.	1.9	15
57	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.	0.2	14
58	Asymmetric Biomimetic Oxidations of Phenols: The Mechanism of the Diastereo- and Enantioselective Synthesis of Thomasidioic Acid. Molecules, 2008, 13, 129-148.	1.7	14
59	Reactivation of the Ready and Unready Oxidized States of [NiFe]-Hydrogenases: Mechanistic Insights from DFT Calculations. Inorganic Chemistry, 2019, 58, 279-293.	1.9	14
60	Tetrameric Silver(I) Complex with Bridging N-Heterocyclic Carbene Ligands: [(iPrIm)Ag(NO3)]4. Organometallics, 2014, 33, 5610-5613.	1.1	12
61	A new multivalent cluster: synthesis, electrochemistry, solid state structure and computational studies on the ironâ€“nickel mixed-metal nitride anions [Fe6Ni6N2(CO)24]nâ€“ (n=2â€“4). Comptes Rendus Chimie, 2005, 8, 1850-1855.	0.2	11
62	Structural variations, electrochemical properties and computational studies on monomeric and dimeric Feâ€“Cu carbide clusters, forming copper-based staple arrays. Dalton Transactions, 2011, 40, 5464.	1.6	11
63	Does the environment around the H-cluster allow coordination of the pendant amine to the catalytic iron center in [FeFe]Âhydrogenases? Answers from theory. Journal of Biological Inorganic Chemistry, 2013, 18, 693-700.	1.1	11
64	A New FeMo Complex as a Model of Heterobimetallic Assemblies in Natural Systems: MÃ¶ssbauer and Density Functional Theory Investigations. Inorganic Chemistry, 2014, 53, 11345-11347.	1.9	11
65	Theoretical investigation of aerobic and anaerobic oxidative inactivation of the [NiFe]-hydrogenase active site. Physical Chemistry Chemical Physics, 2018, 20, 1693-1706.	1.3	11
66	Probing the Effects of Oneâ€Electron Reduction and Protonation on the Electronic Properties of the Feâ€S Clusters in the Activeâ€Ready Form of [FeFe]â€Hydrogenases. A QM/MM Investigation.. ChemPhysChem, 2011, 12, 3376-3382.	1.0	10
67	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,) Tj ETQq1 1 0.784314 rgBT /Over	0.8	9
68	N-Aryl Lactams by Regioselective Ozonation of N-Aryl Cyclic Amines. ISRN Organic Chemistry, 2012, 2012, 1-5.	1.0	9
69	Speciation of Copperâ€“Peptide Complexes in Water Solution Using DFTB and DFT Approaches: Case of the [Cu(HGGG)(Py)] Complex. Journal of Physical Chemistry B, 2012, 116, 6250-6260.	1.2	9
70	Theoretical insights into [NiFe]-hydrogenases oxidation resulting in a slowly reactivating inactive state. Journal of Biological Inorganic Chemistry, 2017, 22, 137-151.	1.1	9
71	Quantum Chemical Investigations of Reaction Paths of Metalloenzymes and Biomimetic Models â€“ The Hydrogenase Example. Topics in Current Chemistry, 2006, , 1-46.	4.0	8
72	Computational approaches to shed light on molecular mechanisms in biological processes. Theoretical Chemistry Accounts, 2007, 117, 723-741.	0.5	8

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73	Copper coordination to the putative cell binding site of angiogenin: a DFT investigation. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	8
74	The Challenging in silico Description of Carbon Monoxide Oxidation as Catalyzed by Molybdenum-Copper CO Dehydrogenase. Frontiers in Chemistry, 2018, 6, 630.	1.8	8
75	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.	1.9	7
76	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.	0.8	6
77	Copper ion interaction with the RNase catalytic site fragment of the angiogenin protein: an experimental and theoretical investigation. Dalton Transactions, 2017, 46, 8524-8538.	1.6	6
78	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.	1.1	6
79	'Measuring' Electron Delocalization in Ï€-Conjugated Systems. Chimia, 2005, 59, 539-544.	0.3	5
80	The regiochemistry of the NO3-promoted gas phase nitration of toluene and phenol with NO2. Journal of Physical Organic Chemistry, 2006, 19, 570-578.	0.9	5
81	Theoretical Insights into the Aerobic Hydrogenase Activity of Molybdenumâ€“Copper CO Dehydrogenase. Inorganics, 2019, 7, 135.	1.2	5
82	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, 8551-8554.	2.2	4
83	Quantum Mechanical Methods for the Investigation of Metalloproteins and Related Bioinorganic Compounds. Methods in Molecular Biology, 2014, 1122, 207-268.	0.4	2
84	Podophyllotoxin and Antitumor Synthetic Aryltetralines. Toward a Biomimetic Preparation. , 2010, , .		1
85	Copper coordination to the putative cell binding site of angiogenin: a DFT investigation. Highlights in Theoretical Chemistry, 2013, , 255-269.	0.0	1