Giuseppe Zampella

List of Publications by Year
in descending order

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100	3,947	109264	133188
papers	citations	35 h-index	59 g-index

104	104	104	3197
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Noncompetitive allosteric inhibitors of the inflammatory chemokine receptors CXCR1 and CXCR2: Prevention of reperfusion injury. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 11791-11796.	3.3	310
2	Density functional study of structural and electronic properties of bimetallic silverâ€“gold clusters: Comparison with pure gold and silver clusters. Journal of Chemical Physics, 2002, 117, 3120-3131.	1.2	305
3	Chelate Control of Diiron(I) Dithiolates Relevant to the [Feâ”Fe]- Hydrogenase Active Site. Inorganic Chemistry, 2007, 46, 1655-1664.	1.9	151
4	Ligand versus Metal Protonation of an Iron Hydrogenase Active Site Mimic. Chemistry - A European Journal, 2007, 13, 7075-7084.	1.7	132
5	DFT investigations of models related to the active site of [NiFe] and [Fe] hydrogenases. Coordination Chemistry Reviews, 2005, 249, 1620-1640.	9.5	123
6	Terminal vs Bridging Hydrides of Diiron Dithiolates: Protonation of Fe₂(dithiolate)(CO)₂(PMe₃)₄. Journal of the American Chemical Society, 2012, 134, 19260-19269.	6.6	117
7	2-Arylpropionic CXC Chemokine Receptor 1 (CXCR1) Ligands as Novel Noncompetitive CXCL8 Inhibitors. Journal of Medicinal Chemistry, 2005, 48, 4312-4331.	2.9	115
8	Reactivity of Peroxo Forms of the Vanadium Haloperoxidase Cofactor. A DFT Investigation. Journal of the American Chemical Society, 2005, 127, 953-960.	6.6	107
9	Redox and Structural Properties of Mixed-Valence Models for the Active Site of the [FeFe]-Hydrogenase: Progress and Challenges. Inorganic Chemistry, 2008, 47, 7405-7414.	1.9	101
10	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
11	Lactate production yield from engineered yeasts is dependent from the host background, the lactate dehydrogenase source and the lactate export. Microbial Cell Factories, 2006, 5, 4.	1.9	84
12	Diiron Dithiolato Carbonyls Related to the H_{ox}^{CO} State of [FeFe]-Hydrogenase. Journal of the American Chemical Society, 2008, 130, 5293-5301.	6.6	80
13	Proton Reduction and Dihydrogen Oxidation on Models of the [2Fe]HCluster of [Fe] Hydrogenases. A Density Functional Theory Investigation. Inorganic Chemistry, 2006, 45, 4109-4118.	1.9	76
14	Insight into the Catalytic Mechanism of Vanadium Haloperoxidases. DFT Investigation of Vanadium Cofactor Reactivity. Inorganic Chemistry, 2006, 45, 7133-7143.	1.9	71
15	Glycine- and Sarcosine-Based Models of Vanadate-Dependent Haloperoxidases in Sulfoxygenation Reactions. Inorganic Chemistry, 2007, 46, 196-207.	1.9	70
16	Isomerization of the hydride complexes [HFe₂(SR)₂(PR₃)x(CO)_{6â”x}]⁺(x = 2, 3, 4) relevant to the active site models for the [FeFe]-hydrogenases. Dalton Transactions, 2010, 39, 3011-3019.	1.6	69
17	Unsensitized Photochemical Hydrogen Production Catalyzed by Diiron Hydrides. Journal of the American Chemical Society, 2012, 134, 4525-4528.	6.6	69
18	Diferrous Cyanides as Models for the Fe-only Hydrogenases. Journal of the American Chemical Society, 2005, 127, 11010-11018.	6.6	68

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19	Theoretical Study of Hydration of Cyanamide and Carbodiimide. Journal of Physical Chemistry A, 2003, 107, 1188-1196.	1.1	62
20	Crystallographic Characterization of a Fully Rotated, Basic Diiron Dithiolate: Model for the H_{red} State?. Chemistry - A European Journal, 2013, 19, 15476-15479.	1.7	61
21	Quantum Mechanical Models of the Resting State of the Vanadium-Dependent Haloperoxidase. Inorganic Chemistry, 2004, 43, 4127-4136.	1.9	58
22	Desymmetrized Diiron Azadithiolato Carbonyls: A Step Toward Modeling the Iron-Only Hydrogenases. Organometallics, 2008, 27, 119-125.	1.1	58
23	New Fe^Iâ€“Fe^I Complex Featuring a Rotated Conformation Related to the [2â€‰Fe]_H Subsite of [Feâ€“Fe] Hydrogenase. Chemistry - A European Journal, 2013, 19, 15458-15461.	1.7	56
24	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
25	Lewis vs. BrÃ¸nsted-basicities of diiron dithiolates: spectroscopic detection of the â€œrotated structureâ€• and remarkable effects of ethane- vs. propanedithiolate. Chemical Communications, 2007, , 2019-2021.	2.2	50
26	Electrochemical and Theoretical Investigations of the Role of the Appended Base on the Reduction of Protons by		

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37	Mechanistic Insight into Electrocatalytic H₂ Production by [Fe₂(CN){Î¼-CN(Me)₂}(Î¼-CO)(CO)(Cp)₂]: Effects of Dithiolate Replacement in [FeFe] Hydrogenase Models. Inorganic Chemistry, 2017, 56, 13852-13864.	1.9	35
38	The ATP-bound conformation of the Mre11â€“Rad50 complex is essential for Tel1/ATM activation. Nucleic Acids Research, 2019, 47, 3550-3567.	6.5	35
39	Photocatalytic Hydrogen Evolution Driven by [FeFe] Hydrogenase Models Tethered to Fluorene and Silafluorene Sensitizers. Chemistry - A European Journal, 2017, 23, 334-345.	1.7	34
40	Structurally distinct Mre11 domains mediate MRX functions in resection, end-tethering and DNA damage resistance. Nucleic Acids Research, 2018, 46, 2990-3008.	6.5	34
41	Oxidatively Induced Reactivity of [Fe₂(CO)₄(Îº²-dppe)(Î¼-pdt)]: an Electrochemical and Theoretical Study of the Structure Change and Ligand Binding Processes. Inorganic Chemistry, 2011, 50, 12575-12585.	1.9	33
42	A Practical Synthesis of 7-Azaindolylcarboxy-endo-tropanamide (DF 1012). Organic Process Research and Development, 2003, 7, 209-213.	1.3	32
43	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
44	Investigation on the Protonation of a Trisubstituted [Fe₂(CO)₃(PPh₃)(Îº²-phen)(Î¼-pdt)] Complex: Rotated versus Unrotated Intermediate Pathways. Inorganic Chemistry, 2010, 49, 5003-5008.	1.9	31
45	Copper reduction and dioxygen activation in Cuâ€“amyloid beta peptide complexes: insight from molecular modelling. Metallomics, 2018, 10, 1618-1630.	1.0	31
46	Functional and structural insights into the MRX/MRN complex, a key player in recognition and repair of DNA double-strand breaks. Computational and Structural Biotechnology Journal, 2020, 18, 1137-1152.	1.9	31
47	Siliconâ€“Heteroaromatic [FeFe] Hydrogenase Model Complexes: Insight into Protonation, Electrochemical Properties, and Molecular Structures. Chemistry - A European Journal, 2015, 21, 5061-5073.	1.7	30
48	[FeFe]â€Hydrogenase Models and Hydrogen: Oxidative Addition of Dihydrogen and Silanes. Angewandte Chemie - International Edition, 2008, 47, 9756-9759.	7.2	28
49	Contrasting Protonation Behavior of Diphosphido vs Dithiolato Diiron(I) Carbonyl Complexes. Organometallics, 2013, 32, 232-238.	1.1	27
50	On the generation of OHÂ· radical species from H2O2 by Cu(I) amyloid beta peptide model complexes: a DFT investigation. Journal of Biological Inorganic Chemistry, 2016, 21, 197-212.	1.1	26
51	Proton Shuttle Mediated by (SCH₂)₂Pâ•O Moiety in [FeFe]-Hydrogenase Mimics: Electrochemical and DFT Studies. ACS Catalysis, 2021, 11, 7080-7098.	5.5	25
52	Electron-Rich, Diiron Bis(monothiolato) Carbonyls: Câ€“S Bond Homolysis in a Mixed Valence Diiron Dithiolate. Inorganic Chemistry, 2018, 57, 4409-4418.	1.9	23
53	Influence of the basicity of internal bases in diiron model complexes on hydrides formation and their transformation into protonated diiron hexacarbonyl form. Journal of Organometallic Chemistry, 2010, 695, 721-729.	0.8	22
54	Structural characterization of the nitrogenase molybdenum-iron protein with the substrate acetylene trapped near the active site. Journal of Inorganic Biochemistry, 2018, 180, 129-134.	1.5	21

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55	DFT investigation of copperâ€“peptide complexes related to the octarepeat domain of the prion protein. Inorganic Chemistry Communication, 2003, 6, 650-653.	1.8	20
56	Excited State Properties of Diiron Dithiolate Hydrides: Implications in the Unsensitized Photocatalysis of H₂ Evolution. Inorganic Chemistry, 2013, 52, 9826-9841.	1.9	20
57	Preparation and Protonation of Fe₂(pdt)(CNR)₆, Electron-Rich Analogues of Fe₂(pdt)(CO)₆. Inorganic Chemistry, 2016, 55, 3401-3412.	1.9	20
58	Bromoperoxidase activity of amavadin dissected: a DFT investigation. Chemical Communications, 2014, 50, 304-307.	2.2	17
59	A rare bond between a soft metal (FeI) and a relatively hard base (ROâ¯, R = phenolic moiety). Inorganic Chemistry Communication, 2010, 13, 1089-1092.	1.8	16
60	Effect of Pyramidalization of the M₂(SR)₂ Center: The Case of (C₅H₅)₂Ni₂(SR)₂. Organometallics, 2016, 35, 836-846.	1.1	16
61	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
62	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
63	Influence of the Dithiolate Bridge on the Oxidative Processes of Diiron Models Related to the Active Site of [FeFe] Hydrogenases. Chemistry - A European Journal, 2017, 23, 4364-4372.	1.7	15
64	Electrochemical and Theoretical Investigations of the Oxidatively Induced Reactivity of the Complex [Fe₂(CO)₄(Îº²â€dmpe)(Î¼â€adt^{Bn})] Related to the Active Site of [FeFe] Hydrogenases. Chemistry - A European Journal, 2018, 24, 15036-15051.	1.7	15
65	Synthetic Designs and Structural Investigations of Biomimetic Niâ€“Fe Thiolates. Inorganic Chemistry, 2019, 58, 2430-2443.	1.9	15
66	Catalytic H2 evolution/oxidation in [FeFe]-hydrogenase biomimetics: account from DFT on the interplay of related issues and proposed solutions. New Journal of Chemistry, 2020, 44, 17596-17615.	1.4	15
67	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
68	Molecular insight into substrate recognition by human cytosolic sialidase NEU2. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1123-1132.	1.5	14
69	Synthesis, characterisation of two hexa-iron clusters with {Fe2S2(CO)x} (x=5 or 6) fragments and investigation into their inter-conversion. Journal of Organometallic Chemistry, 2008, 693, 3751-3759.	0.8	13
70	A Diferrous Dithiolate as a Model of the Elusive H_{ox}^{inact} State of the [FeFe] Hydrogenases: An Electrochemical and Theoretical Dissection of Its Redox Chemistry. Inorganic Chemistry, 2015, 54, 299-311.	1.9	12
71	Imine-Centered Reactions in Imino-Phosphine Complexes of Iron Carbonyls. Organometallics, 2016, 35, 2782-2792.	1.1	12
72	Characterization of a Borane Ïƒ Complex of a Diiron Dithiolate: Model for an Elusive Dihydrogen Adduct. Organometallics, 2017, 36, 2054-2057.	1.1	11

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73	Rational Design of Fe₂(Î¼â€PR₂)₂(L)₆ Coordination Compounds Featuring Tailored Potential Inversion. ChemPhysChem, 2020, 21, 2279-2292.	1.0	11
74	DFT characterization of key intermediates in thiols oxidation catalyzed by amavadin. Dalton Transactions, 2011, 40, 7704.	1.6	10
75	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
76	On the photochemistry of Fe₂(edt)(CO)₄(PMe₃)₂, a [FeFe]â€hydrogenase model: A DFT/TDDFT investigation. International Journal of Quantum Chemistry, 2018, 118, e25537.	1.0	9
77	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
78	Understanding the Mechanism of Vanadium-Dependent Haloperoxidases and Related Biomimetic Catalysis. ACS Symposium Series, 2007, , 148-162.	0.5	8
79	Computational approaches to shed light on molecular mechanisms in biological processes. Theoretical Chemistry Accounts, 2007, 117, 723-741.	0.5	8
80	Stereochemistry of electrophilic attack at 34eâ" dimetallic complexes: the case of diiron dithiolato carbonyls + MeS+. Chemical Communications, 2011, 47, 6554.	2.2	8
81	The reactions of pyridinyl thioesters with triiron dodecacarbonyl: their novel diiron carbonyl complexes and mechanistic investigations. Dalton Transactions, 2012, 41, 9482.	1.6	8
82	Copper coordination to the putative cell binding site of angiogenin: a DFT investigation. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	8
83	Reductive Behavior of [Fe₂(CO)₄(Îº²â€dmpe){Î¼â€(SCH₂)₂NBn}]: Effect of Symmetrization on the Rotated Conformation in Fe^Iâ€Fe^I Models of [2Fe]_H Subsite of [Feâ€Fe]ÂH₂ases. European Journal of Inorganic Chemistry,	1.0	8
84	Insights into the Twoâ€Electron Reductive Process of [FeFe]H₂ase Biomimetics: Cyclic Voltammetry and DFT Investigation on Chelate Control of Redox Properties of [Fe₂(CO)₄(Îº²â€Chelate)(Î¼â€Dithiolate)]. Chemistry - A European Journal, 2020, 26, 17536-17545.	1.7	8
85	On the importance of cyanide in diiron bridging carbyne complexes, unconventional [FeFe]-hydrogenase mimics without dithiolate: An electrochemical and DFT investigation. Inorganica Chimica Acta, 2020, 510, 119745.	1.2	8
86	Straightforward synthesis of novel Akt inhibitors based on a glucose scaffold. Carbohydrate Research, 2010, 345, 1291-1298.	1.1	7
87	DNA binding modes influence Rap1 activity in the regulation of telomere length and MRX functions at DNA ends. Nucleic Acids Research, 2020, 48, 2424-2441.	6.5	7
88	On the propagation of the OH radical produced by Cu-amyloid beta peptide model complexes. Insight from molecular modelling. Metallomics, 2020, 12, 1765-1780.	1.0	7
89	Geometrical influence on the non-biomimetic heterolytic splitting of H₂ by bio-inspired [FeFe]-hydrogenase complexes: a rare example of inverted frustrated Lewis pair based reactivity. Chemical Science, 2022, 13, 4863-4873.	3.7	6
90	Toward Diiron Dithiolato Biomimetics with Rotated Conformation of the [FeFe]â€Hydrogenase Active Site: A DFT Case Study on Electronâ€Rich, Isocyanideâ€Based Scaffolds. European Journal of Inorganic Chemistry, 2022, 2022, .	1.0	4

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91	Superoxide Reduction by Cuâ€Amyloid Beta Peptide Complexes: A Density Functional Theory Study. European Journal of Inorganic Chemistry, 2022, 2022, .	1.0	4
92	Towards hydrophobic carminic acid derivatives and their incorporation in polyacrylates. Royal Society Open Science, 2018, 5, 172399.	1.1	3
93	The Photochemistry of Fe2(S2C3H6)(CO)6(Âµ-CO) and Its Oxidized Form, Two Simple [FeFe]-Hydrogenase CO-Inhibited Models. A DFT and TDDFT Investigation. Inorganics, 2021, 9, 16.	1.2	3
94	Computational and Experimental Investigations of the Fe₂(Î¼-S₂)/Fe₂(Î¼-S)₂ Equilibrium. Inorganic Chemistry, 2021, 60, 3917-3926.	1.9	3
95	Quantum Mechanical Methods for the Investigation of Metalloproteins and Related Bioinorganic Compounds. Methods in Molecular Biology, 2014, 1122, 207-268.	0.4	2
96	Synthesis, Molecular Modeling and Biological Evaluation of Metabolically Stable Analogues of the Endogenous Fatty Acid Amide Palmitoylethanolamide. International Journal of Molecular Sciences, 2020, 21, 9074.	1.8	1
97	CO substitution by PPh3 in Fe2S2(CO)6 proceeds via a novel Fe2S intermediate. Chemical Communications, 2021, 57, 5079-5081.	2.2	1
98	Copper coordination to the putative cell binding site of angiogenin: a DFT investigation. Highlights in Theoretical Chemistry, 2013, , 255-269.	0.0	1
99	Investigations of the electronic-molecular structure of bio-inorganic systems using modern methods of quantum chemistry. Inorganica Chimica Acta, 2022, 532, 120728.	1.2	1
100	Challenges in the Synthesis of Active Site Mimics for [NiFe]-Hydrogenases. Organometallics, 0, , .	1.1	0