Giuseppe Zampella

List of Publications by Citations

98 papers	3,428 citations	33 h-index	56 g-index
104 ext. papers	3,732 ext. citations	6 avg, IF	4.94 L-index

#	Paper	IF	Citations
98	Density functional study of structural and electronic properties of bimetallic silver–gold clusters: Comparison with pure gold and silver clusters. *Journal of Chemical Physics*, **2002**, 117, 3120-3131	3.9	289
97	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, 11791-6	11.5	270
96	Chelate control of diiron(I) dithiolates relevant to the [Fe-Fe]- hydrogenase active site. *Inorganic Chemistry*, **2007**, 46, 1655-64	5.1	140
95	Ligand versus metal protonation of an iron hydrogenase active site mimic. *Chemistry - A European Journal*, **2007**, 13, 7075-84	4.8	124
94	DFT investigations of models related to the active site of [NiFe] and [Fe] hydrogenases. *Coordination Chemistry Reviews*, **2005**, 249, 1620-1640	23.2	120
93	2-Arylpropionic CXC chemokine receptor 1 (CXCR1) ligands as novel noncompetitive CXCL8 inhibitors. *Journal of Medicinal Chemistry*, **2005**, 48, 4312-31	8.3	112
92	Terminal vs bridging hydrides of diiron dithiolates: protonation of Fe2(dithiolate)(CO)2(PMe3)4. *Journal of the American Chemical Society*, **2012**, 134, 19260-9	16.4	106
91	Reactivity of peroxo forms of the vanadium haloperoxidase cofactor. A DFT investigation. *Journal of the American Chemical Society*, **2005**, 127, 953-60	16.4	98
90	Redox and structural properties of mixed-valence models for the active site of the [FeFe]-hydrogenase: progress and challenges. *Inorganic Chemistry*, **2008**, 47, 7405-14	5.1	92
89	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
88	Diiron dithiolato carbonyls related to the H(ox)CO state of [FeFe]-hydrogenase. *Journal of the American Chemical Society*, **2008**, 130, 5293-301	16.4	75
87	Proton reduction and dihydrogen oxidation on models of the [2Fe]H cluster of [Fe] hydrogenases. A density functional theory investigation. *Inorganic Chemistry*, **2006**, 45, 4109-18	5.1	75
86	Glycine- and sarcosine-based models of vanadate-dependent haloperoxidases in sulfoxygenation reactions. *Inorganic Chemistry*, **2007**, 46, 196-207	5.1	69
85	Isomerization of the hydride complexes [HFe2(SR)2(PR3)(x)(CO)(6-x)]+ (x = 2, 3, 4) relevant to the active site models for the [FeFe]-hydrogenases. *Dalton Transactions*, **2010**, 39, 3011-9	4.3	66
84	Insight into the catalytic mechanism of vanadium haloperoxidases. DFT investigation of vanadium cofactor reactivity. *Inorganic Chemistry*, **2006**, 45, 7133-43	5.1	66
83	Diferrous cyanides as models for the Fe-only hydrogenases. *Journal of the American Chemical Society*, **2005**, 127, 11010-8	16.4	65
82	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	6.4	65

81	Unsensitized photochemical hydrogen production catalyzed by diiron hydrides. *Journal of the American Chemical Society*, **2012**, 134, 4525-8	16.4	64
80	Desymmetrized Diiron Azadithiolato Carbonyls: A Step Toward Modeling the Iron-Only Hydrogenases. *Organometallics*, **2008**, 27, 119-125	3.8	57
79	Theoretical Study of Hydration of Cyanamide and Carbodiimide. *Journal of Physical Chemistry A*, **2003**, 107, 1188-1196	2.8	56
78	Quantum mechanical models of the resting state of the vanadium-dependent haloperoxidase. *Inorganic Chemistry*, **2004**, 43, 4127-36	5.1	54
77	Crystallographic characterization of a fully rotated, basic diiron dithiolate: model for the H(red) state?. *Chemistry - A European Journal*, **2013**, 19, 15476-9	4.8	52
76	New Fe(I) -Fe(I) complex featuring a rotated conformation related to the [2 Fe](H) subsite of [Fe-Fe] hydrogenase. *Chemistry - A European Journal*, **2013**, 19, 15458-61	4.8	49
75	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
74	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
73	New reactions of terminal hydrides on a diiron dithiolate. *Journal of the American Chemical Society*, **2014**, 136, 5773-82	16.4	42
72	Lewis vs. Brønsted-basicities of diiron dithiolates: spectroscopic detection of the "rotated structure" and remarkable effects of ethane- vs. propanedithiolate. *Chemical Communications*, **2007**, 2019-21	5.8	42
71	Electrochemical and theoretical investigations of the role of the appended base on the reduction of protons by [Fe2(CO)4(κ2-PNP(R)κS(CH2)3S] (PNP(R) ={Ph2PCH2}2NR, R=Me, Ph). *Chemistry - A European Journal*, **2012**, 18, 11123-38	4.8	38
70	Unveiling how stereoelectronic factors affect kinetics and thermodynamics of protonation regiochemistry in [FeFe] hydrogenase synthetic models: a DFT investigation. *Journal of the American Chemical Society*, **2009**, 131, 10909-17	16.4	38
69	The importance of stereochemically active lone pairs for influencing Pb(II) and As(III) protein binding. *Chemistry - A European Journal*, **2012**, 18, 2040-50	4.8	35
68	Mechanistic Analysis of Nucleophilic Substrates Oxidation by Functional Models of Vanadium-Dependent Haloperoxidases: A Density Functional Theory Study. *European Journal of Inorganic Chemistry*, **2007**, 2007, 515-523	2.3	35
67	DFT dissection of the reduction step in H2 catalytic production by [FeFe]-hydrogenase-inspired models: can the bridging hydride become more reactive than the terminal isomer?. *Inorganic Chemistry*, **2015**, 54, 9529-42	5.1	34
66	DFT characterization of the reaction pathways for terminal- to μ-hydride isomerisation in synthetic models of the [FeFe]-hydrogenase active site. *Chemical Communications*, **2010**, 46, 8824-6	5.8	34
65	Electrochemical and Theoretical Studies of the Impact of the Chelating Ligand on the Reactivity of [Fe2(CO)4(κ2-LL)(μ-pdt)]+Complexes with Different Substrates (LL = IMe-CH2-IMe, dppe; IMe= 1-Methylimidazol-2-ylidene). *Organometallics*, **2012**, 31, 1082-1091	3.8	31
64	Evidence for the formation of a Mo-H intermediate in the catalytic cycle of formate dehydrogenase. *Inorganic Chemistry*, **2012**, 51, 8331-9	5.1	30

63	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
62	Photocatalytic Hydrogen Evolution Driven by [FeFe] Hydrogenase Models Tethered to Fluorene and Silafluorene Sensitizers. *Chemistry - A European Journal*, **2017**, 23, 334-345	4.8	28
61	A sterically stabilized FeI-FeI semi-rotated conformation of [FeFe] hydrogenase subsite model. *Dalton Transactions*, **2015**, 44, 1690-9	4.3	28
60	A Practical Synthesis of 7-Azaindolylcarboxy-endo-tropanamide (DF 1012). *Organic Process Research and Development*, **2003**, 7, 209-213	3.9	28
59	Oxidatively induced reactivity of [Fe2(CO)4(2-dppe)(pdt)]: an electrochemical and theoretical study of the structure change and ligand binding processes. *Inorganic Chemistry*, **2011**, 50, 12575-85	5.1	26
58	The ATP-bound conformation of the Mre11-Rad50 complex is essential for Tel1/ATM activation. *Nucleic Acids Research*, **2019**, 47, 3550-3567	20.1	26
57	Silicon-Heteroaromatic [FeFe] hydrogenase model complexes: insight into protonation, electrochemical properties, and molecular structures. *Chemistry - A European Journal*, **2015**, 21, 5061-73	4.8	25
56	Investigation on the protonation of a trisubstituted [Fe(2)(CO)(3)(PPh(3))(kappa(2)-phen)(mu-pdt)] complex: rotated versus unrotated intermediate pathways. *Inorganic Chemistry*, **2010**, 49, 5003-8	5.1	25
55	[FeFe]-hydrogenase models and hydrogen: oxidative addition of dihydrogen and silanes. *Angewandte Chemie - International Edition*, **2008**, 47, 9756-9	16.4	24
54	Mechanistic Insight into Electrocatalytic H Production by [Fe(CN){CN(Me)}(CO)(CO)(Cp)]: Effects of Dithiolate Replacement in [FeFe] Hydrogenase Models. *Inorganic Chemistry*, **2017**, 56, 13852-13864	5.1	23
53	Contrasting Protonation Behavior of Diphosphido vs Dithiolato Diiron(I) Carbonyl Complexes. *Organometallics*, **2013**, 32, 232-238	3.8	23
52	Structurally distinct Mre11 domains mediate MRX functions in resection, end-tethering and DNA damage resistance. *Nucleic Acids Research*, **2018**, 46, 2990-3008	20.1	20
51	DFT investigation of copper peptide complexes related to the octarepeat domain of the prion protein. *Inorganic Chemistry Communication*, **2003**, 6, 650-653	3.1	20
50	Copper reduction and dioxygen activation in Cu-amyloid beta peptide complexes: insight from molecular modelling. *Metallomics*, **2018**, 10, 1618-1630	4.5	20
49	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	6.8	19
48	On the generation of OH() radical species from H2O2 by Cu(I) amyloid beta peptide model complexes: a DFT investigation. *Journal of Biological Inorganic Chemistry*, **2016**, 21, 197-212	3.7	19
47	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	2.3	19
46	Electron-Rich, Diiron Bis(monothiolato) Carbonyls: C-S Bond Homolysis in a Mixed Valence Diiron Dithiolate. *Inorganic Chemistry*, **2018**, 57, 4409-4418	5.1	17

45	Excited state properties of diiron dithiolate hydrides: implications in the unsensitized photocatalysis of H2 evolution. *Inorganic Chemistry*, **2013**, 52, 9826-41	5.1	17
44	Preparation and Protonation of Fe2(pdt)(CNR)6, Electron-Rich Analogues of Fe2(pdt)(CO)6. *Inorganic Chemistry*, **2016**, 55, 3401-12	5.1	16
43	Bromoperoxidase activity of amavadin dissected: a DFT investigation. *Chemical Communications*, **2014**, 50, 304-7	5.8	14
42	Molecular insight into substrate recognition by human cytosolic sialidase NEU2. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 1123-32	4.2	14
41	A rare bond between a soft metal (FeI) and a relatively hard base (RO□R = phenolic moiety). *Inorganic Chemistry Communication*, **2010**, 13, 1089-1092	3.1	14
40	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	2.3	13
39	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
38	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	4.8	12
37	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
36	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	4.2	10
35	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
34	Characterization of a Borane Complex of a Diiron Dithiolate: Model for an Elusive Dihydrogen Adduct. *Organometallics*, **2017**, 36, 2054-2057	3.8	9
33	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	5.1	9
32	Effect of Pyramidalization of the M2(SR)2Center: The Case of (C5H5)2Ni2(SR)2. *Organometallics*, **2016**, 35, 836-846	3.8	9
31	Electrochemical and Theoretical Investigations of the Oxidatively Induced Reactivity of the Complex [Fe (CO) (□dmpe)(□adt)] Related to the Active Site of [FeFe] Hydrogenases. *Chemistry - A European Journal*, **2018**, 24, 15036-15051	4.8	9
30	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
29	DFT characterization of key intermediates in thiols oxidation catalyzed by amavadin. *Dalton Transactions*, **2011**, 40, 7704-12	4.3	9
28	Reductive Behavior of [Fe2(CO)4(□-dmpe){□(SCH2)2NBn}]: Effect of Symmetrization on the Rotated Conformation in FeI-FeI Models of [2Fe]H Subsite of [Fe-Fe]□H2ases. *European Journal of Inorganic Chemistry*, **2014**, 2014, 3456-3461	2.3	8

27	Copper coordination to the putative cell binding site of angiogenin: a DFT investigation. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	8
26	Computational approaches to shed light on molecular mechanisms in biological processes. *Theoretical Chemistry Accounts*, **2007**, 117, 723-741	1.9	8
25	Understanding the Mechanism of Vanadium-Dependent Haloperoxidases and Related Biomimetic Catalysis. *ACS Symposium Series*, **2007**, 148-162	0.4	8
24	Synthetic Designs and Structural Investigations of Biomimetic Ni-Fe Thiolates. *Inorganic Chemistry*, **2019**, 58, 2430-2443	5.1	7
23	Imine-Centered Reactions in Imino-Phosphine Complexes of Iron Carbonyls. *Organometallics*, **2016**, 35, 2782-2792	3.8	7
22	The reactions of pyridinyl thioesters with triiron dodecacarbonyl: their novel diiron carbonyl complexes and mechanistic investigations. *Dalton Transactions*, **2012**, 41, 9482-92	4.3	7
21	Stereochemistry of electrophilic attack at 34e? dimetallic complexes: the case of diiron dithiolato carbonyls + MeS+. *Chemical Communications*, **2011**, 47, 6554-6	5.8	7
20	Quantum Chemical Investigations of Reaction Paths of Metalloenzymes and Biomimetic Models The Hydrogenase Example. *Topics in Current Chemistry*, **2006**, 1-46		7
19	On the photochemistry of Fe2(edt)(CO)4(PMe3)2, a [FeFe]-hydrogenase model: A DFT/TDDFT investigation. *International Journal of Quantum Chemistry*, **2018**, 118, e25537	2.1	7
18	[FeFe]-Hydrogenase Models and Hydrogen: Oxidative Addition of Dihydrogen and Silanes. *Angewandte Chemie*, **2008**, 120, 9902-9905	3.6	6
17	Rational Design of Fe (PR) (L) Coordination Compounds Featuring Tailored Potential Inversion. *ChemPhysChem*, **2020**, 21, 2279-2292	3.2	6
16	Straightforward synthesis of novel Akt inhibitors based on a glucose scaffold. *Carbohydrate Research*, **2010**, 345, 1291-8	2.9	5
15	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	3.6	5
14	Proton Shuttle Mediated by (SCH2)2P?O Moiety in [FeFe]-Hydrogenase Mimics: Electrochemical and DFT Studies. *ACS Catalysis*, **2021**, 11, 7080-7098	13.1	5
13	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	2.7	3
12	On the propagation of the OH radical produced by Cu-amyloid beta peptide model complexes. Insight from molecular modelling. *Metallomics*, **2020**, 12, 1765-1780	4.5	2
11	Quantum mechanical methods for the investigation of metalloproteins and related bioinorganic compounds. *Methods in Molecular Biology*, **2014**, 1122, 207-68	1.4	2
10	Insights into the Two-Electron Reductive Process of [FeFe]H ase Biomimetics: Cyclic Voltammetry and DFT Investigation on Chelate Control of Redox Properties of [Fe (CO) (-Chelate)(Dithiolate)]. *Chemistry - A European Journal*, **2020**, 26, 17536-17545	4.8	2

9	Hydrogenases: Theoretical Investigations Towards Bioinspired H2 Production and Activation **2009**,		1
8	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	20.1	1
7	Synthesis, Molecular Modeling and Biological Evaluation of Metabolically Stable Analogues of the Endogenous Fatty Acid Amide Palmitoylethanolamide. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	1
6	Computational and Experimental Investigations of the Fe(ES)/Fe(ES) Equilibrium. *Inorganic Chemistry*, **2021**, 60, 3917-3926	5.1	1
5	The Photochemistry of Fe2(S2C3H6)(CO)6(μ-CO) and Its Oxidized Form, Two Simple [FeFe]-Hydrogenase CO-Inhibited Models. A DFT and TDDFT Investigation. *Inorganics*, **2021**, 9, 16	2.9	1
4	Towards hydrophobic carminic acid derivatives and their incorporation in polyacrylates. *Royal Society Open Science*, **2018**, 5, 172399	3.3	1
3	Copper coordination to the putative cell binding site of angiogenin: a DFT investigation. *Highlights in Theoretical Chemistry*, **2013**, 255-269		0
2	Investigations of the electronic-molecular structure of bio-inorganic systems using modern methods of quantum chemistry. *Inorganica Chimica Acta*, **2022**, 532, 120728	2.7	
1	CO substitution by PPh in FeS(CO) proceeds via a novel FeS intermediate. *Chemical Communications* , **2021**, 57, 5079-5081	5.8	