

Giuseppe Zampella

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Investigations of the electronic-molecular structure of bio-inorganic systems using modern methods of quantum chemistry. <i>Inorganica Chimica Acta</i> , 2022 , 532, 120728	2.7	
97	Computational and Experimental Investigations of the Fe(II)/Fe(III) Equilibrium. <i>Inorganic Chemistry</i> , 2021 , 60, 3917-3926	5.1	1
96	Proton Shuttle Mediated by (SCH ₂) ₂ P=O Moiety in [FeFe]-Hydrogenase Mimics: Electrochemical and DFT Studies. <i>ACS Catalysis</i> , 2021 , 11, 7080-7098	13.1	5
95	CO substitution by PPh in FeS(CO) proceeds via a novel FeS intermediate. <i>Chemical Communications</i> , 2021 , 57, 5079-5081	5.8	
94	The Photochemistry of Fe ₂ (S ₂ C ₃ H ₆)(CO) ₆ (η -CO) and Its Oxidized Form, Two Simple [FeFe]-Hydrogenase CO-Inhibited Models. A DFT and TDDFT Investigation. <i>Inorganics</i> , 2021 , 9, 16	2.9	1
93	Functional and structural insights into the MRX/MRN complex, a key player in recognition and repair of DNA double-strand breaks. <i>Computational and Structural Biotechnology Journal</i> , 2020 , 18, 1137-1152	6.8	19
92	On the propagation of the OH radical produced by Cu-amyloid beta peptide model complexes. Insight from molecular modelling. <i>Metallomics</i> , 2020 , 12, 1765-1780	4.5	2
91	On the importance of cyanide in diiron bridging carbyne complexes, unconventional [FeFe]-hydrogenase mimics without dithiolate: An electrochemical and DFT investigation. <i>Inorganica Chimica Acta</i> , 2020 , 510, 119745	2.7	3
90	DNA binding modes influence Rap1 activity in the regulation of telomere length and MRX functions at DNA ends. <i>Nucleic Acids Research</i> , 2020 , 48, 2424-2441	20.1	1
89	Synthesis, Molecular Modeling and Biological Evaluation of Metabolically Stable Analogues of the Endogenous Fatty Acid Amide Palmitoylethanolamide. <i>International Journal of Molecular Sciences</i> , 2020 , 21,	6.3	1
88	Catalytic H ₂ evolution/oxidation in [FeFe]-hydrogenase biomimetics: account from DFT on the interplay of related issues and proposed solutions. <i>New Journal of Chemistry</i> , 2020 , 44, 17596-17615	3.6	5
87	Insights into the Two-Electron Reductive Process of [FeFe]H ₂ ase Biomimetics: Cyclic Voltammetry and DFT Investigation on Chelate Control of Redox Properties of [Fe(CO) ₂ (η -Chelate)(η -Dithiolate)]. <i>Chemistry - A European Journal</i> , 2020 , 26, 17536-17545	4.8	2
86	Rational Design of Fe(II) Coordination Compounds Featuring Tailored Potential Inversion. <i>ChemPhysChem</i> , 2020 , 21, 2279-2292	3.2	6
85	Synthetic Designs and Structural Investigations of Biomimetic Ni-Fe Thiolates. <i>Inorganic Chemistry</i> , 2019 , 58, 2430-2443	5.1	7
84	The ATP-bound conformation of the Mre11-Rad50 complex is essential for Tel1/ATM activation. <i>Nucleic Acids Research</i> , 2019 , 47, 3550-3567	20.1	26
83	H ₂ Activation in [FeFe]-Hydrogenase Cofactor Versus Diiron Dithiolate Models: Factors Underlying the Catalytic Success of Nature and Implications for an Improved Biomimicry. <i>Chemistry - A European Journal</i> , 2019 , 25, 1227-1241	4.8	12
82	Electron-Rich, Diiron Bis(monothiolato) Carbonyls: C-S Bond Homolysis in a Mixed Valence Diiron Dithiolate. <i>Inorganic Chemistry</i> , 2018 , 57, 4409-4418	5.1	17

81	Structurally distinct Mre11 domains mediate MRX functions in resection, end-tethering and DNA damage resistance. <i>Nucleic Acids Research</i> , 2018 , 46, 2990-3008	20.1	20
80	Structural characterization of the nitrogenase molybdenum-iron protein with the substrate acetylene trapped near the active site. <i>Journal of Inorganic Biochemistry</i> , 2018 , 180, 129-134	4.2	10
79	Electrochemical and Theoretical Investigations of the Oxidatively Induced Reactivity of the Complex [Fe (CO) (η^5 -dmpe)(η^5 -edt)] Related to the Active Site of [FeFe] Hydrogenases. <i>Chemistry - A European Journal</i> , 2018 , 24, 15036-15051	4.8	9
78	On the photochemistry of Fe ₂ (edt)(CO) ₄ (PMe ₃) ₂ , a [FeFe]-hydrogenase model: A DFT/TDDFT investigation. <i>International Journal of Quantum Chemistry</i> , 2018 , 118, e25537	2.1	7
77	Copper reduction and dioxygen activation in Cu-amyloid beta peptide complexes: insight from molecular modelling. <i>Metallomics</i> , 2018 , 10, 1618-1630	4.5	20
76	Towards hydrophobic carminic acid derivatives and their incorporation in polyacrylates. <i>Royal Society Open Science</i> , 2018 , 5, 172399	3.3	1
75	Photocatalytic Hydrogen Evolution Driven by [FeFe] Hydrogenase Models Tethered to Fluorene and Silafluorene Sensitizers. <i>Chemistry - A European Journal</i> , 2017 , 23, 334-345	4.8	28
74	Characterization of a Borane Complex of a Diiron Dithiolate: Model for an Elusive Dihydrogen Adduct. <i>Organometallics</i> , 2017 , 36, 2054-2057	3.8	9
73	Influence of the Dithiolate Bridge on the Oxidative Processes of Diiron Models Related to the Active Site of [FeFe] Hydrogenases. <i>Chemistry - A European Journal</i> , 2017 , 23, 4364-4372	4.8	12
72	Mechanistic Insight into Electrocatalytic H ₂ Production by [Fe(CN){ECN(Me)}{ECO}(CO)(Cp)]: Effects of Dithiolate Replacement in [FeFe] Hydrogenase Models. <i>Inorganic Chemistry</i> , 2017 , 56, 13852-13864	5.1	23
71	Imine-Centered Reactions in Imino-Phosphine Complexes of Iron Carbonyls. <i>Organometallics</i> , 2016 , 35, 2782-2792	3.8	7
70	On the generation of OH(\cdot) radical species from H ₂ O ₂ by Cu(I) amyloid beta peptide model complexes: a DFT investigation. <i>Journal of Biological Inorganic Chemistry</i> , 2016 , 21, 197-212	3.7	19
69	Effect of Pyramidalization of the M ₂ (SR) ₂ Center: The Case of (C ₅ H ₅) ₂ Ni ₂ (SR) ₂ . <i>Organometallics</i> , 2016 , 35, 836-846	3.8	9
68	Preparation and Protonation of Fe ₂ (pdt)(CNR) ₆ , Electron-Rich Analogues of Fe ₂ (pdt)(CO) ₆ . <i>Inorganic Chemistry</i> , 2016 , 55, 3401-12	5.1	16
67	Silicon-Heteroaromatic [FeFe] hydrogenase model complexes: insight into protonation, electrochemical properties, and molecular structures. <i>Chemistry - A European Journal</i> , 2015 , 21, 5061-73	4.8	25
66	A sterically stabilized FeI-FeI semi-rotated conformation of [FeFe] hydrogenase subsite model. <i>Dalton Transactions</i> , 2015 , 44, 1690-9	4.3	28
65	DFT dissection of the reduction step in H ₂ catalytic production by [FeFe]-hydrogenase-inspired models: can the bridging hydride become more reactive than the terminal isomer?. <i>Inorganic Chemistry</i> , 2015 , 54, 9529-42	5.1	34
64	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. <i>Inorganic Chemistry</i> , 2015 , 54, 299-311	5.1	9

63	Bromoperoxidase activity of amavadin dissected: a DFT investigation. <i>Chemical Communications</i> , 2014 , 50, 304-7	5.8	14
62	New reactions of terminal hydrides on a diiron dithiolate. <i>Journal of the American Chemical Society</i> , 2014 , 136, 5773-82	16.4	42
61	Towards biomimetic models of the reduced [FeFe]-hydrogenase that preserve the key structural features of the enzyme active site; a DFT investigation. <i>International Journal of Hydrogen Energy</i> , 2014 , 39, 18565-18573	6.7	10
60	Reductive Behavior of [Fe ₂ (CO) ₄ (η-dmpe){η-[S(CH ₂) ₂ NBn]}]: Effect of Symmetrization on the Rotated Conformation in Fe-Fe Models of [2Fe]H Subsite of [Fe-Fe]H ₂ ases. <i>European Journal of Inorganic Chemistry</i> , 2014 , 2014, 3456-3461	2.3	8
59	Quantum mechanical methods for the investigation of metalloproteins and related bioinorganic compounds. <i>Methods in Molecular Biology</i> , 2014 , 1122, 207-68	1.4	2
58	Contrasting Protonation Behavior of Diphosphido vs Dithiolato Diiron(I) Carbonyl Complexes. <i>Organometallics</i> , 2013 , 32, 232-238	3.8	23
57	Excited state properties of diiron dithiolate hydrides: implications in the unsensitized photocatalysis of H ₂ evolution. <i>Inorganic Chemistry</i> , 2013 , 52, 9826-41	5.1	17
56	Crystallographic characterization of a fully rotated, basic diiron dithiolate: model for the H(red) state?. <i>Chemistry - A European Journal</i> , 2013 , 19, 15476-9	4.8	52
55	New Fe(I) -Fe(I) complex featuring a rotated conformation related to the [2 Fe](H) subsite of [Fe-Fe] hydrogenase. <i>Chemistry - A European Journal</i> , 2013 , 19, 15458-61	4.8	49
54	Copper coordination to the putative cell binding site of angiogenin: a DFT investigation. <i>Highlights in Theoretical Chemistry</i> , 2013 , 255-269		0
53	The importance of stereochemically active lone pairs for influencing Pb(II) and As(III) protein binding. <i>Chemistry - A European Journal</i> , 2012 , 18, 2040-50	4.8	35
52	The reactions of pyridinyl thioesters with triiron dodecacarbonyl: their novel diiron carbonyl complexes and mechanistic investigations. <i>Dalton Transactions</i> , 2012 , 41, 9482-92	4.3	7
51	Speciation of copper-peptide complexes in water solution using DFTB and DFT approaches: case of the [Cu(HGGG)(Py)] complex. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 6250-60	3.4	9
50	Terminal vs bridging hydrides of diiron dithiolates: protonation of Fe ₂ (dithiolate)(CO) ₂ (PMe ₃) ₄ . <i>Journal of the American Chemical Society</i> , 2012 , 134, 19260-9	16.4	106
49	Evidence for the formation of a Mo-H intermediate in the catalytic cycle of formate dehydrogenase. <i>Inorganic Chemistry</i> , 2012 , 51, 8331-9	5.1	30
48	Molecular insight into substrate recognition by human cytosolic sialidase NEU2. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012 , 80, 1123-32	4.2	14
47	Unsensitized photochemical hydrogen production catalyzed by diiron hydrides. <i>Journal of the American Chemical Society</i> , 2012 , 134, 4525-8	16.4	64
46	Electrochemical and Theoretical Studies of the Impact of the Chelating Ligand on the Reactivity of [Fe ₂ (CO) ₄ (η-LL)(η-pdt)] ⁺ Complexes with Different Substrates (LL = IMe-CH ₂ -IMe, dppe; IMe = 1-Methylimidazol-2-ylidene). <i>Organometallics</i> , 2012 , 31, 1082-1091	3.8	31

45	Electrochemical and theoretical investigations of the role of the appended base on the reduction of protons by $[\text{Fe}_2(\text{CO})_4(\eta\text{-PNP}(\text{R})(\text{E}(\text{CH}_2)_3\text{S}))]$ ($\text{PNP}(\text{R}) = \{\text{Ph}_2\text{PCH}_2\}_2\text{NR}$, $\text{R} = \text{Me}, \text{Ph}$). <i>Chemistry - A European Journal</i> , 2012 , 18, 11123-38	4.8	38
44	Copper coordination to the putative cell binding site of angiogenin: a DFT investigation. <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	8
43	Oxidatively induced reactivity of $[\text{Fe}_2(\text{CO})_4(\eta\text{-dppe})(\text{E}(\text{pdt}))]$: an electrochemical and theoretical study of the structure change and ligand binding processes. <i>Inorganic Chemistry</i> , 2011 , 50, 12575-85	5.1	26
42	Stereochemistry of electrophilic attack at 34e ⁻ dimetallic complexes: the case of diiron dithiolato carbonyls + MeS^+ . <i>Chemical Communications</i> , 2011 , 47, 6554-6	5.8	7
41	DFT characterization of key intermediates in thiols oxidation catalyzed by amavadin. <i>Dalton Transactions</i> , 2011 , 40, 7704-12	4.3	9
40	Investigation on the protonation of a trisubstituted $[\text{Fe}_2(\text{CO})_3(\text{PPh}_3)(\kappa^2\text{-phen})(\mu\text{-pdt})]$ complex: rotated versus unrotated intermediate pathways. <i>Inorganic Chemistry</i> , 2010 , 49, 5003-8	5.1	25
39	Isomerization of the hydride complexes $[\text{HFe}_2(\text{SR})_2(\text{PR}_3)_x(\text{CO})_{(6-x)}]^+$ ($x = 2, 3, 4$) relevant to the active site models for the $[\text{FeFe}]$ -hydrogenases. <i>Dalton Transactions</i> , 2010 , 39, 3011-9	4.3	66
38	DFT characterization of the reaction pathways for terminal- to η hydride isomerisation in synthetic models of the $[\text{FeFe}]$ -hydrogenase active site. <i>Chemical Communications</i> , 2010 , 46, 8824-6	5.8	34
37	Influence of the basicity of internal bases in diiron model complexes on hydrides formation and their transformation into protonated diiron hexacarbonyl form. <i>Journal of Organometallic Chemistry</i> , 2010 , 695, 721-729	2.3	19
36	Straightforward synthesis of novel Akt inhibitors based on a glucose scaffold. <i>Carbohydrate Research</i> , 2010 , 345, 1291-8	2.9	5
35	A rare bond between a soft metal (FeI) and a relatively hard base ($\text{RO}\ddot{\text{O}}\text{R} = \text{phenolic moiety}$). <i>Inorganic Chemistry Communication</i> , 2010 , 13, 1089-1092	3.1	14
34	Unveiling how stereoelectronic factors affect kinetics and thermodynamics of protonation regiochemistry in $[\text{FeFe}]$ hydrogenase synthetic models: a DFT investigation. <i>Journal of the American Chemical Society</i> , 2009 , 131, 10909-17	16.4	38
33	Hydrogenases: Theoretical Investigations Towards Bioinspired H ₂ Production and Activation 2009 ,		1
32	Redox and structural properties of mixed-valence models for the active site of the $[\text{FeFe}]$ -hydrogenase: progress and challenges. <i>Inorganic Chemistry</i> , 2008 , 47, 7405-14	5.1	92
31	Desymmetrized Diiron Azadithiolato Carbonyls: A Step Toward Modeling the Iron-Only Hydrogenases. <i>Organometallics</i> , 2008 , 27, 119-125	3.8	57
30	Diiron dithiolato carbonyls related to the $\text{H}(\text{ox})\text{CO}$ state of $[\text{FeFe}]$ -hydrogenase. <i>Journal of the American Chemical Society</i> , 2008 , 130, 5293-301	16.4	75
29	$[\text{FeFe}]$ -hydrogenase models and hydrogen: oxidative addition of dihydrogen and silanes. <i>Angewandte Chemie - International Edition</i> , 2008 , 47, 9756-9	16.4	24
28	$[\text{FeFe}]$ -Hydrogenase Models and Hydrogen: Oxidative Addition of Dihydrogen and Silanes. <i>Angewandte Chemie</i> , 2008 , 120, 9902-9905	3.6	6

27	Synthesis, characterisation of two hexa-iron clusters with $\{\text{Fe}_2\text{S}_2(\text{CO})_x\}$ ($x = 5$ or 6) fragments and investigation into their inter-conversion. <i>Journal of Organometallic Chemistry</i> , 2008 , 693, 3751-3759	2.3	13
26	A DFT investigation on structural and redox properties of a synthetic Fe_6S_6 assembly closely related to the $[\text{FeFe}]$ -hydrogenases active site. <i>Comptes Rendus Chimie</i> , 2008 , 11, 834-841	2.7	13
25	Insights into the mechanism of electrocatalytic hydrogen evolution mediated by $\text{Fe}_2(\text{S}_2\text{C}_3\text{H}_6)(\text{CO})_6$: the simplest functional model of the Fe-hydrogenase active site. <i>Inorganic Chemistry</i> , 2007 , 46, 108-16	5.1	77
24	Lewis vs. Brønsted-basicities of diiron dithiolates: spectroscopic detection of the "rotated structure" and remarkable effects of ethane- vs. propanedithiolate. <i>Chemical Communications</i> , 2007 , 2019-21	5.8	42
23	Chelate control of diiron(II) dithiolates relevant to the $[\text{Fe-Fe}]$ - hydrogenase active site. <i>Inorganic Chemistry</i> , 2007 , 46, 1655-64	5.1	140
22	Glycine- and sarcosine-based models of vanadate-dependent haloperoxidases in sulfoxxygenation reactions. <i>Inorganic Chemistry</i> , 2007 , 46, 196-207	5.1	69
21	Ligand versus metal protonation of an iron hydrogenase active site mimic. <i>Chemistry - A European Journal</i> , 2007 , 13, 7075-84	4.8	124
20	Mechanistic Analysis of Nucleophilic Substrates Oxidation by Functional Models of Vanadium-Dependent Haloperoxidases: A Density Functional Theory Study. <i>European Journal of Inorganic Chemistry</i> , 2007 , 2007, 515-523	2.3	35
19	Computational approaches to shed light on molecular mechanisms in biological processes. <i>Theoretical Chemistry Accounts</i> , 2007 , 117, 723-741	1.9	8
18	Understanding the Mechanism of Vanadium-Dependent Haloperoxidases and Related Biomimetic Catalysis. <i>ACS Symposium Series</i> , 2007 , 148-162	0.4	8
17	Quantum Chemical Investigations of Reaction Paths of Metalloenzymes and Biomimetic Models □ The Hydrogenase Example. <i>Topics in Current Chemistry</i> , 2006 , 1-46		7
16	Lactate production yield from engineered yeasts is dependent from the host background, the lactate dehydrogenase source and the lactate export. <i>Microbial Cell Factories</i> , 2006 , 5, 4	6.4	65
15	Insight into the catalytic mechanism of vanadium haloperoxidases. DFT investigation of vanadium cofactor reactivity. <i>Inorganic Chemistry</i> , 2006 , 45, 7133-43	5.1	66
14	Proton reduction and dihydrogen oxidation on models of the $[\text{2Fe}]_H$ cluster of $[\text{Fe}]$ hydrogenases. A density functional theory investigation. <i>Inorganic Chemistry</i> , 2006 , 45, 4109-18	5.1	75
13	Diferrous cyanides as models for the Fe-only hydrogenases. <i>Journal of the American Chemical Society</i> , 2005 , 127, 11010-8	16.4	65
12	2-Arylpropionic CXC chemokine receptor 1 (CXCR1) ligands as novel noncompetitive CXCL8 inhibitors. <i>Journal of Medicinal Chemistry</i> , 2005 , 48, 4312-31	8.3	112
11	DFT Investigation of H_2 activation by $[\text{M}(\text{NHPnPr}_3)(\text{S}_3\text{Q})]$ ($\text{M} = \text{Ni}, \text{Pd}$). Insight into key factors relevant to the design of hydrogenase functional models. <i>Journal of the American Chemical Society</i> , 2005 , 127, 13180-9	16.4	29
10	Reactivity of peroxo forms of the vanadium haloperoxidase cofactor. A DFT investigation. <i>Journal of the American Chemical Society</i> , 2005 , 127, 953-60	16.4	98

9	DFT investigations of models related to the active site of [NiFe] and [Fe] hydrogenases. <i>Coordination Chemistry Reviews</i> , 2005 , 249, 1620-1640	23.2	120
8	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. <i>Chemistry - A European Journal</i> , 2005 , 11, 509-20	4.8	43
7	Noncompetitive allosteric inhibitors of the inflammatory chemokine receptors CXCR1 and CXCR2: prevention of reperfusion injury. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2004 , 101, 11791-6	11.5	270
6	A theoretical study of spin states in Ni-S4 complexes and models of the [NiFe] hydrogenase active site. <i>Journal of Biological Inorganic Chemistry</i> , 2004 , 9, 873-84	3.7	47
5	Quantum mechanical models of the resting state of the vanadium-dependent haloperoxidase. <i>Inorganic Chemistry</i> , 2004 , 43, 4127-36	5.1	54
4	DFT investigation of copper-peptide complexes related to the octarepeat domain of the prion protein. <i>Inorganic Chemistry Communication</i> , 2003 , 6, 650-653	3.1	20
3	A Practical Synthesis of 7-Azaindolylcarboxy-endo-tropanamide (DF 1012). <i>Organic Process Research and Development</i> , 2003 , 7, 209-213	3.9	28
2	Theoretical Study of Hydration of Cyanamide and Carbodiimide. <i>Journal of Physical Chemistry A</i> , 2003 , 107, 1188-1196	2.8	56
1	Density functional study of structural and electronic properties of bimetallic silver-gold clusters: Comparison with pure gold and silver clusters. <i>Journal of Chemical Physics</i> , 2002 , 117, 3120-3131	3.9	289