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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.

80 papers	1,864 citations	26 h-index	40 g-index
89 ext. papers	2,065 ext. citations	6.4 avg, IF	4.68 L-index

#	Paper	IF	Citations
80	Investigations of the electronic-molecular structure of bio-inorganic systems using modern methods of quantum chemistry. *Inorganica Chimica Acta*, **2022**, 532, 120728	2.7	
79	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
78	Triiron clusters derived from dinuclear complexes related to the active site of [FeFe] hydrogenases: steric effect of the dithiolate bridge on redox properties, a DFT analysis. *Inorganic Chemistry Frontiers*, **2021**, 8, 3659-3674	6.8	0
77	QM/MM study of the binding of H to MoCu CO dehydrogenase: development and applications of improved H van der Waals parameters. *Journal of Molecular Modeling*, **2021**, 27, 68	2	2
76	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
75	The large subunit of the regulatory [NiFe]-hydrogenase from - a minimal hydrogenase?. *Chemical Science*, **2020**, 11, 5453-5465	9.4	13
74	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
73	Dynamical Behavior and Conformational Selection Mechanism of the Intrinsically Disordered Sic1 Kinase-Inhibitor Domain. *Life*, **2020**, 10,	3	1
72	Rational Design of Fe (IPR) (L) Coordination Compounds Featuring Tailored Potential Inversion. *ChemPhysChem*, **2020**, 21, 2279-2292	3.2	6
71	A thiocarbonate sink on the enzymatic energy landscape of aerobic CO oxidation? Answers from DFT and QM/MM models of MoCu CO-dehydrogenases. *Journal of Catalysis*, **2019**, 372, 201-205	7.3	5
70	Role of the carbon defects in the catalytic oxygen reduction by graphite nanoparticles: a spectromagnetic, electrochemical and computational integrated approach. *Physical Chemistry Chemical Physics*, **2019**, 21, 6021-6032	3.6	16
69	Protonation and electrochemical properties of a bisphosphide diiron hexacarbonyl complex bearing amino groups on the phosphide bridge. *Dalton Transactions*, **2019**, 48, 16595-16603	4.3	5
68	Theoretical Insights into the Aerobic Hydrogenase Activity of Molybdenum Copper CO Dehydrogenase. *Inorganics*, **2019**, 7, 135	2.9	1
67	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
66	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
65	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
64	Interaction of the H-Cluster of FeFe Hydrogenase with Halides. *Journal of the American Chemical Society*, **2018**, 140, 5485-5492	16.4	14

63	The Challenging Description of Carbon Monoxide Oxidation as Catalyzed by Molybdenum-Copper CO Dehydrogenase. *Frontiers in Chemistry*, **2018**, 6, 630	5	3
62	Organophosphorous ligands in hydrogenase-inspired iron-based catalysts: A DFT study on the energetics of metal protonation as a function of P-atom substitution. *Journal of Physical Organic Chemistry*, **2018**, 31, e3748	2.1	3
61	Targeting Amyloid Aggregation: An Overview of Strategies and Mechanisms. *International Journal of Molecular Sciences*, **2018**, 19,	6.3	63
60	Experimental and Theoretical Investigation on the Catalytic Generation of Environmentally Persistent Free Radicals from Benzene. *Journal of Physical Chemistry C*, **2017**, 121, 9381-9393	3.8	24
59	Theoretical and experimental investigation of UV□Vis absorption spectrum in a Eu(3+) based complex for luminescent downshifting applications. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	1
58	Temperature Dependence of the Catalytic Two- versus Four-Electron Reduction of Dioxygen by a Hexanuclear Cobalt Complex. *Journal of the American Chemical Society*, **2017**, 139, 15033-15042	16.4	28
57	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
56	A theoretical study on the reactivity of the Mo/Cu-containing carbon monoxide dehydrogenase with dihydrogen. *Protein Engineering, Design and Selection*, **2017**, 30, 167-172	1.9	5
55	Reactivity of the Excited States of the H-Cluster of FeFe Hydrogenases. *Journal of the American Chemical Society*, **2016**, 138, 13612-13618	16.4	21
54	Computational Insight on CO2 Fixation to Produce Styrene Carbonate Assisted by a Single-Center Aluminum(III) Catalyst and Quaternary Ammonium Salts. *ChemCatChem*, **2016**, 8, 1167-1175	5.2	17
53	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
52	TDDFT modeling of the CO-photolysis of Fe2(S2C3H6)(CO)6, a model of the [FeFe]-hydrogenase catalytic site. *International Journal of Quantum Chemistry*, **2014**, 114, 851-861	2.1	9
51	A conserved loop in polynucleotide phosphorylase (PNPase) essential for both RNA and ADP/phosphate binding. *Biochimie*, **2014**, 97, 49-59	4.6	9
50	Computational Investigation on the Spectroscopic Properties of Thiophene Based Europium □Diketonate Complexes. *Journal of Chemical Theory and Computation*, **2014**, 10, 767-77	6.4	19
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	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
47	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
46	DFT Investigation of Models Related to the Active Siteof Hydrogenases **2014**, 137-160		0

45	The oxidative inactivation of FeFe hydrogenase reveals the flexibility of the H-cluster. *Nature Chemistry*, **2014**, 6, 336-42	17.6	75
44	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
43	New Systematic Route to Mixed-Valence Triiron Clusters Derived from Dinuclear Models of the Active Site of [FeFe]-Hydrogenases. *Organometallics*, **2014**, 33, 6290-6293	3.8	8
42	Quantum mechanical methods for the investigation of metalloproteins and related bioinorganic compounds. *Methods in Molecular Biology*, **2014**, 1122, 207-68	1.4	2
41	H2 binding and splitting on a new-generation [FeFe]-hydrogenase model featuring a redox-active decamethylferrocenyl phosphine ligand: a theoretical investigation. *Inorganic Chemistry*, **2013**, 52, 1901-8	5.1	26
40	Towards [NiFe]-hydrogenase biomimetic models that couple H2 binding with functionally relevant intramolecular electron transfers: a quantum chemical study. *Dalton Transactions*, **2013**, 42, 13845-54	4.3	7
39	Access to a Cu(II)-O-Cu(II) motif: spectroscopic properties, solution structure, and reactivity. *Journal of the American Chemical Society*, **2013**, 135, 16148-60	16.4	42
38	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
37	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
36	Regulation of hSos1 activity is a system-level property generated by its multi-domain structure. *Biotechnology Advances*, **2012**, 30, 154-68	17.8	7
35	Lewis acid trapping of an elusive copper-tosylnitrene intermediate using scandium triflate. *Journal of the American Chemical Society*, **2012**, 134, 14710-3	16.4	99
34	BLUF hydrogen network dynamics and UV/Vis spectra: a combined molecular dynamics and quantum chemical study. *Journal of Computational Chemistry*, **2012**, 33, 2233-42	3.5	11
33	Synthesis and Spectroscopic Characterisation of a Heterodinuclear Iron(III)-Copper(II) Complex Based on an Asymmetric Dinucleating Ligand System. *European Journal of Inorganic Chemistry*, **2012** , 2012, 4565-4569	2.3	8
32	Copper coordination to the putative cell binding site of angiogenin: a DFT investigation. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	8
31	CO disrupts the reduced H-cluster of FeFe hydrogenase. A combined DFT and protein film voltammetry study. *Journal of the American Chemical Society*, **2011**, 133, 2096-9	16.4	58
30	A theoretical study on the enhancement of functionally relevant electron transfers in biomimetic models of [FeFe]-hydrogenases. *Inorganic Chemistry*, **2011**, 50, 6987-95	5.1	29
29	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
28	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

27	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
26	Targeting intermediates of [FeFe]-hydrogenase by CO and CN vibrational signatures. *Inorganic Chemistry*, **2011**, 50, 3888-900	5.1	48
25	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
24	CO Affinity and Bonding Properties of [FeFe] Hydrogenase Active Site Models. A DFT Study. *Organometallics*, **2010**, 29, 2013-2025	3.8	27
23	Quantum refinement of [FeFe] hydrogenase indicates a dithiomethylamine ligand. *Journal of the American Chemical Society*, **2010**, 132, 4512-3	16.4	70
22	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
21	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
20	Fast generation of broken-symmetry states in a large system including multiple iron□sulfur assemblies: Investigation of QM/MM energies, clusters charges, and spin populations. *International Journal of Quantum Chemistry*, **2010**, 111, n/a-n/a	2.1	17
19	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
18	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
17	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
16	Optical and structural properties of copper-oxytocin dications in the gas phase. *Journal of Physical Chemistry B*, **2009**, 113, 11293-300	3.4	28
15	DFT/TDDFT exploration of the potential energy surfaces of the ground state and excited states of Fe2(S2C3H6)(CO)6: a simple functional model of the [FeFe] hydrogenase active site. *Journal of Physical Chemistry A*, **2009**, 113, 5657-70	2.8	29
14	Hydrogenases: Theoretical Investigations Towards Bioinspired H2 Production and Activation **2009**,		1
13	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
12	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
11	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
10	A QM/MM investigation of the activation and catalytic mechanism of Fe-only hydrogenases. *Inorganic Chemistry*, **2007**, 46, 5911-21	5.1	109

9	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
8	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
7	Influence of a Large 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
6	Genetic analysis of polynucleotide phosphorylase structure and functions. *Biochimie*, **2007**, 89, 145-57	4.6	44
5	Quantum Chemical Investigations of Reaction Paths of Metalloenzymes and Biomimetic Models The Hydrogenase Example. *Topics in Current Chemistry*, **2006**, 1-46		7
4	Time-dependent density functional theory study of Fe2(CO)9 low-lying electronic excited states. *Journal of Physical Chemistry A*, **2006**, 110, 12900-7	2.8	14
3	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
2	In silico functional characterization of a double histone fold domain from the Heliothis zea virus 1. *BMC Bioinformatics*, **2005**, 6 Suppl 4, S15	3.6	5
1	Identification and in silico analysis of a new group of double-histone fold-containing proteins. *Journal of Molecular Modeling*, **2005**, 12, 76-84	2	3