

Luca Bertini

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.

66

papers

1,599

citations

22

h-index

38

g-index

74

ext. papers

1,788

ext. citations

5.2

avg. IF

4.47

L-index

#	Paper	IF	Citations
66	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	
65	Mechanism of Hydrogen Sulfide-Dependent Inhibition of FeFe Hydrogenase. <i>ACS Catalysis</i> , 2021 , 11, 15162-15176	13.1	1
64	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
63	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. <i>Inorganic Chemistry</i> , 2021 , 60, 387-402	5.1	8
62	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. <i>Inorganic Chemistry Frontiers</i> , 2021 , 8, 3659-3674	6.8	0
61	The Photochemistry of Fe ₂ (S ₂ C ₃ H ₆)(CO) ₆ (μ-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
60	Photochemistry and photoinhibition of the H-cluster of FeFe hydrogenases. <i>Sustainable Energy and Fuels</i> , 2021 , 5, 4248-4260	5.8	2
59	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
58	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
57	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
56	Rational Design of Fe (EPR) (L) Coordination Compounds Featuring Tailored Potential Inversion. <i>ChemPhysChem</i> , 2020 , 21, 2279-2292	3.2	6
55	Synthetic Designs and Structural Investigations of Biomimetic Ni-Fe Thiolates. <i>Inorganic Chemistry</i> , 2019 , 58, 2430-2443	5.1	7
54	Anomalous Intrinsic Fluorescence of HCl and NaOH Aqueous Solutions. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 7230-7236	6.4	9
53	H 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
52	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
51	Interaction of the H-Cluster of FeFe Hydrogenase with Halides. <i>Journal of the American Chemical Society</i> , 2018 , 140, 5485-5492	16.4	14
50	Electrochemical and Theoretical Investigations of the Oxidatively Induced Reactivity of the Complex [Fe(CO)(dmpe)(adt)] Related to the Active Site of [FeFe] Hydrogenases. <i>Chemistry - A European Journal</i> , 2018 , 24, 15036-15051	4.8	9

49	Catalytic Mechanism of Fungal Lytic Polysaccharide Monooxygenases Investigated by First-Principles Calculations. <i>Inorganic Chemistry</i> , 2018 , 57, 86-97	5.1	54
48	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
47	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
46	Towards hydrophobic carminic acid derivatives and their incorporation in polyacrylates. <i>Royal Society Open Science</i> , 2018 , 5, 172399	3.3	1
45	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
44	Photophysical Properties of S, Se and Te-Substituted Deoxyguanosines: Insight into Their Ability To Act as Chemotherapeutic Agents. <i>Journal of Chemical Information and Modeling</i> , 2017 , 57, 234-242	6.1	22
43	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
42	Photoinhibition of FeFe Hydrogenase. <i>ACS Catalysis</i> , 2017 , 7, 7378-7387	13.1	13
41	Mechanistic Insight into Electrocatalytic H ₂ Production by [Fe(CN){ECN(Me)}(CO)(CO)(Cp)]: Effects of Dithiolate Replacement in [FeFe] Hydrogenase Models. <i>Inorganic Chemistry</i> , 2017 , 56, 13852-13864	5.1	23
40	Reactivity of the Excited States of the H-Cluster of FeFe Hydrogenases. <i>Journal of the American Chemical Society</i> , 2016 , 138, 13612-13618	16.4	21
39	On the generation of OH(II) 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
38	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
37	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
36	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
35	A sterically stabilized FeI-FeI semi-rotated conformation of [FeFe] hydrogenase subsite model. <i>Dalton Transactions</i> , 2015 , 44, 1690-9	4.3	28
34	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
33	TDDFT modeling of the CO-photolysis of Fe ₂ (S ₂ C ₃ H ₆)(CO) ₆ , a model of the [FeFe]-hydrogenase catalytic site. <i>International Journal of Quantum Chemistry</i> , 2014 , 114, 851-861	2.1	9
32	Computational Investigation on the Spectroscopic Properties of Thiophene Based Europium EDiketonate Complexes. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 767-77	6.4	19

31	Bromoperoxidase activity of amavadin dissected: a DFT investigation. <i>Chemical Communications</i> , 2014 , 50, 304-7	5.8	14
30	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
29	Inhibitors of the Cdc34 acidic loop: A computational investigation integrating molecular dynamics, virtual screening and docking approaches. <i>FEBS Open Bio</i> , 2014 , 4, 473-84	2.7	8
28	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
27	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
26	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
25	Unsensitized photochemical hydrogen production catalyzed by diiron hydrides. <i>Journal of the American Chemical Society</i> , 2012 , 134, 4525-8	16.4	64
24	Copper coordination to the putative cell binding site of angiogenin: a DFT investigation. <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	8
23	CO disrupts the reduced H-cluster of FeFe hydrogenase. A combined DFT and protein film voltammetry study. <i>Journal of the American Chemical Society</i> , 2011 , 133, 2096-9	16.4	58
22	DFT characterization of key intermediates in thiols oxidation catalyzed by amavadin. <i>Dalton Transactions</i> , 2011 , 40, 7704-12	4.3	9
21	On the Photochemistry of the Low-Lying Excited State of Fe ₂ (CO) ₆ S ₂ . A DFT and QTAIM Investigation. <i>Organometallics</i> , 2011 , 30, 487-498	3.8	19
20	CO Affinity and Bonding Properties of [FeFe] Hydrogenase Active Site Models. A DFT Study. <i>Organometallics</i> , 2010 , 29, 2013-2025	3.8	27
19	Functionally relevant interplay between the Fe(4)S(4) cluster and CN(-) ligands in the active site of [FeFe]-hydrogenases. <i>Journal of the American Chemical Society</i> , 2010 , 132, 4992-3	16.4	31
18	DFT/TDDFT exploration of the potential energy surfaces of the ground state and excited states of Fe ₂ (S ₂ C ₃ H ₆)(CO) ₆ : a simple functional model of the [FeFe] hydrogenase active site. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 5657-70	2.8	29
17	Hydrogenases: Theoretical Investigations Towards Bioinspired H ₂ Production and Activation 2009 ,		1
16	Insights into the mechanism of electrocatalytic hydrogen evolution mediated by Fe ₂ (S ₂ C ₃ H ₆)(CO) ₆ : the simplest functional model of the Fe-hydrogenase active site. <i>Inorganic Chemistry</i> , 2007 , 46, 108-16	5.1	77
15	Structure and energetics of Fe ₂ (CO) ₈ singlet and triplet electronic states. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 12152-62	2.8	15
14	Electronic structure of the Co ₄ Sn ₆ Te ₆ ternary skutterudite phase. <i>Physica Status Solidi - Rapid Research Letters</i> , 2007 , 1, 244-246	2.5	7

13	Chemical insight into electron density and wave functions: software developments and applications to crystals, molecular complexes and materials science. <i>Theoretical Chemistry Accounts</i> , 2007 , 117, 847-884	1.9	45
12	Time-dependent density functional theory study of Fe ₂ (CO) ₉ low-lying electronic excited states. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 12900-7	2.8	14
11	Nanostructured Co _{1-x} Ni _x (Sb _{1-y} Te _y) ₃ skutterudites: Theoretical modeling, synthesis and thermoelectric properties. <i>Journal of Applied Physics</i> , 2005 , 97, 044317	2.5	68
10	A Chemical Approach to the First-Principles Modeling of Novel Thermoelectric Materials 2005 , 7-1-7-13		1
9	The local form of the source function as a fingerprint of strong and weak intra- and intermolecular interactions. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2004 , 60, 438-49		62
8	Interstitial Zn atoms do the trick in thermoelectric zinc antimonide, Zn ₄ Sb ₃ : a combined maximum entropy method X-ray electron density and ab initio electronic structure study. <i>Chemistry - A European Journal</i> , 2004 , 10, 3861-70	4.8	151
7	Borromean binding in H ₂ with Yukawa potential: A nonadiabatic quantum Monte Carlo study. <i>Physical Review A</i> , 2004 , 69,	2.6	24
6	The impact of the actual geometrical structure of a thermoelectric material on its electronic transport properties: the case of doped skutterudite systems. <i>Journal of Chemical Physics</i> , 2004 , 121, 8983-9	3.9	50
5	Chemical information from the source function. <i>Journal of Computational Chemistry</i> , 2003 , 24, 422-36	3.5	147
4	Guest-framework interaction in type I inorganic clathrates with promising thermoelectric properties: on the ionic versus neutral nature of the alkaline-earth metal guest A in A ₈ Ga ₁₆ Ge ₃₀ (A=Sr, Ba). <i>Chemistry - A European Journal</i> , 2003 , 9, 4556-68	4.8	64
3	Nanostructured Co _{1-x} Ni _x Sb ₃ skutterudites: Synthesis, thermoelectric properties, and theoretical modeling. <i>Journal of Applied Physics</i> , 2003 , 93, 438-447	2.5	82
2	Explicitly correlated trial wavefunctions in quantum Monte Carlo calculations of excited states of Be and Be ⁻ . <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2001 , 34, 257-266	1.3	12
1	Linear expansions of correlated functions: Variational Monte Carlo case study. <i>International Journal of Quantum Chemistry</i> , 1999 , 74, 23-33	2.1	9