Luca Bertini

List of Publications by Year
in descending order

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71	1,935	257101 24	276539 41
papers	citations	h-index	g-index

74	74	74	1967
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Interstitial Zn Atoms Do the Trick in Thermoelectric Zinc Antimonide, Zn4Sb3: A Combined Maximum Entropy Method X-ray Electron Density and Ab Initio Electronic Structure Study. Chemistry - A European Journal, 2004, 10, 3861-3870.	1.7	169
2	Chemical information from the source function. Journal of Computational Chemistry, 2003, 24, 422-436.	1.5	160
3	Nanostructured Co1â^'xNixSb3 skutterudites: Synthesis, thermoelectric properties, and theoretical modeling. Journal of Applied Physics, 2003, 93, 438-447.	1.1	89
4	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
5	Nanostructured Co1â^'xNix(Sb1â^'yTey)3 skutterudites: Theoretical modeling, synthesis and thermoelectric properties. Journal of Applied Physics, 2005, 97, 044317.	1.1	74
6	Catalytic Mechanism of Fungal Lytic Polysaccharide Monooxygenases Investigated by First-Principles Calculations. Inorganic Chemistry, 2018, 57, 86-97.	1.9	72
7	Guestâ€“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 A8Ga16Ge30 (A=Sr, Ba). Chemistry - A European Journal, 2003, 9, 4556-4568.	1.7	69
8	Unsensitized Photochemical Hydrogen Production Catalyzed by Diiron Hydrides. Journal of the American Chemical Society, 2012, 134, 4525-4528.	6.6	69
9	The local form of the source function as a fingerprint of strong and weak intra- and intermolecular interactions. Acta Crystallographica Section A: Foundations and Advances, 2004, 60, 438-449.	0.3	66
10	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, 2096-2099.	6.6	62
11	The impact of the actual geometrical structure of a thermoelectric material on its electronic transport properties: The case of doped skutterudite systems. Journal of Chemical Physics, 2004, 121, 8983-8989.	1.2	51
12	Chemical insight into electron density and wave functions: software developments and applications to crystals, molecular complexes and materials science. Theoretical Chemistry Accounts, 2007, 117, 847-884.	0.5	48
13	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, 9529-9542.	1.9	38
14	A sterically stabilized Fe^Iâ€“Fe^I semi-rotated conformation of [FeFe] hydrogenase subsite model. Dalton Transactions, 2015, 44, 1690-1699.	1.6	36
15	Photophysical Properties of S, Se and Te-Substituted Deoxyguanosines: Insight into Their Ability To Act as Chemotherapeutic Agents. Journal of Chemical Information and Modeling, 2017, 57, 234-242.	2.5	35
16	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
17	Functionally Relevant Interplay between the Fe₄S₄ Cluster and CN^{â^'} Ligands in the Active Site of [FeFe]-Hydrogenases. Journal of the American Chemical Society, 2010, 132, 4992-4993.	6.6	34
18	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

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19	Copper reduction and dioxygen activation in Cuâ€“amyloid beta peptide complexes: insight from molecular modelling. Metallomics, 2018, 10, 1618-1630.	1.0	31
20	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, 5657-5670.	1.1	30
21	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
22	CO Affinity and Bonding Properties of [FeFe] Hydrogenase Active Site Models. A DFT Study. Organometallics, 2010, 29, 2013-2025.	1.1	28
23	Borromean binding inH2with Yukawa potential: A nonadiabatic quantum Monte Carlo study. Physical Review A, 2004, 69, .	1.0	26
24	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
25	Reactivity of the Excited States of the H-Cluster of FeFe Hydrogenases. Journal of the American Chemical Society, 2016, 138, 13612-13618.	6.6	25
26	Interaction of the H-Cluster of FeFe Hydrogenase with Halides. Journal of the American Chemical Society, 2018, 140, 5485-5492.	6.6	25
27	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
28	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
29	Excited State Properties of Diiron Dithiolate Hydrides: Implications in the Unsensitized Photocatalysis of H₂ Evolution. Inorganic Chemistry, 2013, 52, 9826-9841.	1.9	20
30	Computational Investigation on the Spectroscopic Properties of Thiophene Based Europium Î²-Diketonate Complexes. Journal of Chemical Theory and Computation, 2014, 10, 767-777.	2.3	20
31	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
32	On the Photochemistry of the Low-Lying Excited State of Fe₂(CO)₆S₂. A DFT and QTAIM Investigation. Organometallics, 2011, 30, 487-498.	1.1	19
33	Bromoperoxidase activity of amavadin dissected: a DFT investigation. Chemical Communications, 2014, 50, 304-307.	2.2	17
34	Photoinhibition of FeFe Hydrogenase. ACS Catalysis, 2017, 7, 7378-7387.	5.5	17
35	Time-Dependent Density Functional Theory Study of Fe2(CO)9Low-Lying Electronic Excited States. Journal of Physical Chemistry A, 2006, 110, 12900-12907.	1.1	16
36	Structure and Energetics of Fe2(CO)8Singlet and Triplet Electronic States. Journal of Physical Chemistry A, 2007, 111, 12152-12162.	1.1	16

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37	Effect of Pyramidalization of the M₂(SR)₂ Center: The Case of (C₅H₅)₂Ni₂(SR)₂. Organometallics, 2016, 35, 836-846.	1.1	16
38	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
39	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
40	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
41	Electrochemical and Theoretical Investigations of the Oxidatively Induced Reactivity of the Complex [Fe₂(CO)₄(Î¼²â€dmpe)(Î¼â€adt^{Bn})] Related to the Active Site of [FeFe] Hydrogenases. Chemistry - A European Journal, 2018, 24, 15036-15051.	1.7	15
42	Synthetic Designs and Structural Investigations of Biomimetic Niâ€“Fe Thiolates. Inorganic Chemistry, 2019, 58, 2430-2443.	1.9	15
43	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
44	First-Principles Calculations on Ni,Fe-Containing Carbon Monoxide Dehydrogenases Reveal Key Stereoelectronic Features for Binding and Release of CO₂ to/from the C-Cluster. Inorganic Chemistry, 2021, 60, 387-402.	1.9	15
45	Explicitly correlated trial wavefunctions in quantum Monte Carlo calculations of excited states of Be and Be-. Journal of Physics B: Atomic, Molecular and Optical Physics, 2001, 34, 257-266.	0.6	14
46	Mechanism of Hydrogen Sulfide-Dependent Inhibition of FeFe Hydrogenase. ACS Catalysis, 2021, 11, 15162-15176.	5.5	13
47	Anomalous Intrinsic Fluorescence of HCl and NaOH Aqueous Solutions. Journal of Physical Chemistry Letters, 2019, 10, 7230-7236.	2.1	12
48	TDDFT modeling of the COâ€photolysis of Fe₂(S₂C₃H₆)(CO)₆, a model of the [FeFe]â€hydrogenase catalytic site. International Journal of Quantum Chemistry, 2014, 114, 851-861.	1.0	11
49	Rational Design of Fe₂(Î¼â€PR₂)₂(L)₆ Coordination Compounds Featuring Tailored Potential Inversion. ChemPhysChem, 2020, 21, 2279-2292.	1.0	11
50	DFT characterization of key intermediates in thiols oxidation catalyzed by amavadin. Dalton Transactions, 2011, 40, 7704.	1.6	10
51	Linear expansions of correlated functions: Variational Monte Carlo case study. International Journal of Quantum Chemistry, 1999, 74, 23-33.	1.0	9
52	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
53	Inhibitors of the Cdc34 acidic loop: A computational investigation integrating molecular dynamics, virtual screening and docking approaches. FEBS Open Bio, 2014, 4, 473-484.	1.0	9
54	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

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55	Copper coordination to the putative cell binding site of angiogenin: a DFT investigation. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	8
56	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
57	Electronic structure of the Co₄Sn₆Te₆ternary skutterudite phase. Physica Status Solidi - Rapid Research Letters, 2007, 1, 244-246.	1.2	7
58	Photochemistry and photoinhibition of the H-cluster of FeFe hydrogenases. Sustainable Energy and Fuels, 2021, 5, 4248-4260.	2.5	7
59	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
60	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
61	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
62	Superoxide Reduction by Cuâ€Amyloid Beta Peptide Complexes: A Density Functional Theory Study. European Journal of Inorganic Chemistry, 2022, 2022, .	1.0	4
63	Towards hydrophobic carminic acid derivatives and their incorporation in polyacrylates. Royal Society Open Science, 2018, 5, 172399.	1.1	3
64	Triiron clusters derived from dinuclear complexes related to the active site of [Feâ€“Fe] hydrogenases: steric effect of the dithiolate bridge on redox properties, a DFT analysis. Inorganic Chemistry Frontiers, 2021, 8, 3659-3674.	3.0	3
65	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
66	Quantum Mechanical Methods for the Investigation of Metalloproteins and Related Bioinorganic Compounds. Methods in Molecular Biology, 2014, 1122, 207-268.	0.4	2
67	A Chemical Approacht o the First-Principles Modeling of Novel Thermoelectric Materials. , 2005, , 7-1-7-13.		1
68	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
69	Fluorescence of KCl Aqueous Solution: A Possible Spectroscopic Signature of Nucleation. Journal of Physical Chemistry B, 2022, 126, 2564-2572.	1.2	1
70	Guestâ€"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 A8Ga16Ge30 (A:) Tj ETQq0 0 0 rgBT /Overlock 10 T	0	0
71	Challenges in the Synthesis of Active Site Mimics for [NiFe]-Hydrogenases. Organometallics, 0, , .	1.1	0