Luca Bertini

List of Publications by Citations

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	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, 3861-70	4.8	151
65	Chemical information from the source function. *Journal of Computational Chemistry*, **2003**, 24, 422-36	3.5	147
64	Nanostructured Co1−xNixSb3 skutterudites: Synthesis, thermoelectric properties, and theoretical modeling. *Journal of Applied Physics*, **2003**, 93, 438-447	2.5	82
63	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
62	Nanostructured Co1−xNix(Sb1−yTey)3 skutterudites: Theoretical modeling, synthesis and thermoelectric properties. *Journal of Applied Physics*, **2005**, 97, 044317	2.5	68
61	Unsensitized photochemical hydrogen production catalyzed by diiron hydrides. *Journal of the American Chemical Society*, **2012**, 134, 4525-8	16.4	64
60	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 A8Ga16Ge30 (A=Sr, Ba). *Chemistry - A European Journal*, **2003**, 9, 4556-68	4.8	64
59	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, 438-49		62
58	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
57	Catalytic Mechanism of Fungal Lytic Polysaccharide Monooxygenases Investigated by First-Principles Calculations. *Inorganic Chemistry*, **2018**, 57, 86-97	5.1	54
56	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, 8983-9	3.9	50
55	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	1.9	45
54	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
53	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
52	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
51	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
50	A sterically stabilized FeI-FeI semi-rotated conformation of [FeFe] hydrogenase subsite model. *Dalton Transactions*, **2015**, 44, 1690-9	4.3	28

49	CO Affinity and Bonding Properties of [FeFe] Hydrogenase Active Site Models. A DFT Study. *Organometallics*, **2010**, 29, 2013-2025	3.8	27
48	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
47	Borromean binding in H2 with Yukawa potential: A nonadiabatic quantum Monte Carlo study. *Physical Review A*, **2004**, 69,	2.6	24
46	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
45	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	6.1	22
44	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
43	Copper reduction and dioxygen activation in Cu-amyloid beta peptide complexes: insight from molecular modelling. *Metallomics*, **2018**, 10, 1618-1630	4.5	20
42	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
41	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
40	On the Photochemistry of the Low-Lying Excited State of Fe2(CO)6S2. A DFT and QTAIM Investigation. *Organometallics*, **2011**, 30, 487-498	3.8	19
39	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
38	Excited state properties of diiron dithiolate hydrides: implications in the unsensitized photocatalysis of H2 evolution. *Inorganic Chemistry*, **2013**, 52, 9826-41	5.1	17
37	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
36	Structure and energetics of Fe2(CO)8 singlet and triplet electronic states. *Journal of Physical Chemistry A*, **2007**, 111, 12152-62	2.8	15
35	Interaction of the H-Cluster of FeFe Hydrogenase with Halides. *Journal of the American Chemical Society*, **2018**, 140, 5485-5492	16.4	14
34	Bromoperoxidase activity of amavadin dissected: a DFT investigation. *Chemical Communications*, **2014**, 50, 304-7	5.8	14
33	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
32	Photoinhibition of FeFe Hydrogenase. *ACS Catalysis*, **2017**, 7, 7378-7387	13.1	13

31	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
30	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	1.3	12
29	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
28	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
27	Effect of Pyramidalization of the M2(SR)2Center: The Case of (C5H5)2Ni2(SR)2. *Organometallics*, **2016**, 35, 836-846	3.8	9
26	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
25	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
24	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
23	DFT characterization of key intermediates in thiols oxidation catalyzed by amavadin. *Dalton Transactions*, **2011**, 40, 7704-12	4.3	9
22	Linear expansions of correlated functions: Variational Monte Carlo case study. *International Journal of Quantum Chemistry*, **1999**, 74, 23-33	2.1	9
21	Anomalous Intrinsic Fluorescence of HCl and NaOH Aqueous Solutions. *Journal of Physical Chemistry Letters*, **2019**, 10, 7230-7236	6.4	9
20	Inhibitors of the Cdc34 acidic loop: A computational investigation integrating molecular dynamics, virtual screening and docking approaches. *FEBS Open Bio*, **2014**, 4, 473-84	2.7	8
19	Copper coordination to the putative cell binding site of angiogenin: a DFT investigation. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	8
18	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
17	Synthetic Designs and Structural Investigations of Biomimetic Ni-Fe Thiolates. *Inorganic Chemistry*, **2019**, 58, 2430-2443	5.1	7
16	Electronic structure of the Co4Sn6Te6 ternary skutterudite phase. *Physica Status Solidi - Rapid Research Letters*, **2007**, 1, 244-246	2.5	7
15	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
14	Rational Design of Fe (□PR) (L) Coordination Compounds Featuring Tailored Potential Inversion. *ChemPhysChem*, **2020**, 21, 2279-2292	3.2	6

13	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
12	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
11	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
10	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
9	Quantum mechanical methods for the investigation of metalloproteins and related bioinorganic compounds. *Methods in Molecular Biology*, **2014**, 1122, 207-68	1.4	2
8	Photochemistry and photoinhibition of the H-cluster of FeFe hydrogenases. *Sustainable Energy and Fuels*, **2021**, 5, 4248-4260	5.8	2
7	Hydrogenases: Theoretical Investigations Towards Bioinspired H2 Production and Activation **2009**,		1
6	Mechanism of Hydrogen Sulfide-Dependent Inhibition of FeFe Hydrogenase. *ACS Catalysis*, **2021**, 11, 15162-15176	13.1	1
5	A Chemical Approacht o the First-Principles Modeling of Novel Thermoelectric Materials **2005**, 7-1-7-13		1
4	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
3	Towards hydrophobic carminic acid derivatives and their incorporation in polyacrylates. *Royal Society Open Science*, **2018**, 5, 172399	3.3	1
2	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
1	Investigations of the electronic-molecular structure of bio-inorganic systems using modern methods of quantum chemistry. *Inorganica Chimica Acta*, **2022**, 532, 120728	2.7	