Jordi Cirera

List of Publications by Year in Descending Order

52 papers	4,193 citations	26 h-index	59 g-index
59 ext. papers	4,724 ext. citations	8.5 avg, IF	5.49 L-index

#	Paper	IF	Citations
52	Accurate calculation of spin-state energy gaps in Fe(III) spin-crossover systems using density functional methods. *Dalton Transactions*, **2021**, 50, 17635-17642	4.3	1
51	Piano-Stool Ruthenium(II) Complexes with Delayed Cytotoxic Activity: Origin of the Lag Time. *Inorganic Chemistry*, **2021**, 60, 7974-7990	5.1	9
50	Spin-Crossover Properties of an Iron(II) Coordination Nanohoop. *Angewandte Chemie*, **2021**, 133, 3557-3560	3.6	
49	Spin-Crossover Properties of an Iron(II) Coordination Nanohoop. *Angewandte Chemie - International Edition*, **2021**, 60, 3515-3518	16.4	4
48	Controlling the spin-crossover behavior of the [Cr(indenyl)] family ligand functionalization. *Dalton Transactions*, **2021**, 50, 8704-8710	4.3	2
47	[Co/Fe(Alkyl-tpdt)]: Alkyl-Substituted Cobalt and Iron Bis-dithiolenethiophenic Complexes. *Inorganic Chemistry*, **2020**, 59, 9261-9269	5.1	
46	Thermal spin crossover in Fe(ii) and Fe(iii). Accurate spin state energetics at the solid state. *Physical Chemistry Chemical Physics*, **2020**, 22, 4938-4945	3.6	17
45	Coordination control of a semicarbazide Schiff base ligand for spontaneous aggregation of a Ni2Ln2 cubane family: influence of ligand arms and carboxylate bridges on the organization of the magnetic core. *New Journal of Chemistry*, **2020**, 44, 4812-4821	3.6	2
44	Assessment of the SCAN Functional for Spin-State Energies in Spin-Crossover Systems. *Journal of Physical Chemistry A*, **2020**, 124, 5053-5058	2.8	7
43	Electronic Control of Spin-Crossover Properties in Four-Coordinate Bis(formazanate) Iron(II) Complexes. *Journal of the American Chemical Society*, **2020**, 142, 20170-20181	16.4	8
42	Computational assessment on the Tolman cone angles for P-ligands. *Dalton Transactions*, **2019**, 48, 15036-15048	4.3	87
41	Computational Modeling of Transition Temperatures in Spin-Crossover Systems. *Comments on Inorganic Chemistry*, **2019**, 39, 216-241	3.9	14
40	Microwave assisted synthesis of heterometallic 3d-4f MLn complexes. *Dalton Transactions*, **2019**, 48, 12440-12450	4.3	14
39	Electronic and Steric Control of the Spin-Crossover Behavior in [(Cp)Mn] Manganocenes. *Inorganic Chemistry*, **2018**, 57, 702-709	5.1	13
38	Solvation-Guided Design of Fluorescent Probes for Discrimination of Amyloids. *Scientific Reports*, **2018**, 8, 6950	4.9	12
37	Benchmarking Density Functional Methods for Calculation of State Energies of First Row Spin-Crossover Molecules. *Inorganic Chemistry*, **2018**, 57, 14097-14105	5.1	77
36	An Unprecedented Stimuli-Controlled Single-Crystal Reversible Phase Transition of a Metal-Organic Framework and Its Application to a Novel Method of Guest Encapsulation. *Advanced Materials*, **2018**, 30, e1800726	24	25

35	Mercurophilic interactions: a theoretical study on the importance of ligands. *Physical Chemistry Chemical Physics*, **2017**, 19, 11645-11654	3.6	25
34	Structure of the Reduced Copper Active Site in Preprocessed Galactose Oxidase: Ligand Tuning for One-Electron O Activation in Cofactor Biogenesis. *Journal of the American Chemical Society*, **2016**, 138, 13219-13229	16.4	27
33	Ferromagnetism in polynuclear systems based on non-linear [MnII2MnIII] building blocks. *Inorganic Chemistry Frontiers*, **2016**, 3, 1272-1279	6.8	7
32	Electronic Structure Modulation in an Exceptionally Stable Non-Heme Nitrosyl Iron(II) Spin-Crossover Complex. *Chemistry - A European Journal*, **2016**, 22, 12741-51	4.8	13
31	Modeling Magnetic Properties with Density Functional Theory-Based Methods **2016**, 419-446		1
30	Theoretical Modeling of the Ligand-Tuning Effect over the Transition Temperature in Four-Coordinated Fe(II) Molecules. *Inorganic Chemistry*, **2016**, 55, 1657-63	5.1	22
29	Non-Switching 1,2-Dithienylethene-based Diplatinum(II) Complex Showing High Cytotoxicity. *Inorganic Chemistry*, **2016**, 55, 5356-64	5.1	8
28	Molecular Mechanisms of Spin Crossover in the {Fe(pz)[Pt(CN)4]} Metal-Organic Framework upon Water Adsorption. *Journal of the American Chemical Society*, **2016**, 138, 6123-6	16.4	33
27	Theoretical modeling of two-step spin-crossover transitions in FeII dinuclear systems. *Journal of Materials Chemistry C*, **2015**, 3, 7954-7961	7.1	25
26	MIL-101(Fe) as a lithium-ion battery electrode material: a relaxation and intercalation mechanism during lithium insertion. *Journal of Materials Chemistry A*, **2015**, 3, 4738-4744	13	130
25	Copper active sites in biology. *Chemical Reviews*, **2014**, 114, 3659-853	68.1	1040
24	Theoretical modeling of spin crossover in metal-organic frameworks: [Fe(pz)2Pt(CN)4] as a case study. *Inorganic Chemistry*, **2014**, 53, 11020-8	5.1	32
23	Guest effect on spin-crossover frameworks. *Reviews in Inorganic Chemistry*, **2014**, 34, 199-216	2.4	22
22	Spin State and Stereochemistry **2013**, 441-468		2
21	Chemically crosslinked isoreticular metal-organic frameworks. *Chemical Communications*, **2013**, 49, 3200-28		34
20	Stereospinomers of pentacoordinate iron porphyrin complexes: the case of the [Fe(porphyrinato)(CN)]- anions. *Dalton Transactions*, **2013**, 42, 7002-8	4.3	7
19	Theoretical prediction of spin-crossover temperatures in ligand-driven light-induced spin change systems. *Inorganic Chemistry*, **2012**, 51, 8194-201	5.1	75
18	The effects of electronic polarization on water adsorption in metal-organic frameworks: H2O in MIL-53(Cr). *Journal of Chemical Physics*, **2012**, 137, 054704	3.9	43

17	How to build molecules with large magnetic anisotropy. *Chemistry - A European Journal*, **2009**, 15, 4078-87	4.8	139
16	Accurate computed enthalpies of spin crossover in iron and cobalt complexes. *Journal of Physical Chemistry A*, **2009**, 113, 10033-9	2.8	123
15	Can large magnetic anisotropy and high spin really coexist?. *Chemical Communications*, **2008**, 52-4	5.8	184
14	Stereochemistry and spin state in four-coordinate transition metal compounds. *Inorganic Chemistry*, **2008**, 47, 2871-89	5.1	82
13	Spectroscopic and electronic structure studies of phenolate Cu(II) complexes: phenolate ring orientation and activation related to cofactor biogenesis. *Journal of the American Chemical Society*, **2008**, 130, 16262-73	16.4	31
12	Exchange coupling in CuIIGdIII dinuclear complexes: A theoretical perspective. *Comptes Rendus Chimie*, **2008**, 11, 1227-1234	2.7	53
11	Quantitative geometric descriptions of the belt iron atoms of the iron-molybdenum cofactor of nitrogenase and synthetic iron(II) model complexes. *Inorganic Chemistry*, **2007**, 46, 60-71	5.1	40
10	Ferromagnetic coupling in trinuclear, partial cubane Cu(II) complexes with a micro(3)-OH core: magnetostructural correlations. *Chemistry - A European Journal*, **2007**, 13, 9297-309	4.8	67
9	Shape and spin state in four-coordinate transition-metal complexes: the case of the d(6) configuration. *Chemistry - A European Journal*, **2006**, 12, 3162-7	4.8	131
8	How high the spin? Allowed and forbidden spin states in transition-metal chemistry. *Angewandte Chemie - International Edition*, **2006**, 45, 3012-20	16.4	42
7	Hoch oder niedrig? Zur Erlaubtheit von Spinzustänen in der Übergangsmetallchemie. *Angewandte Chemie*, **2006**, 118, 3078-3087	3.6	19
6	Continuous Shape Measures as a Stereochemical Tool in Organometallic Chemistry. *Organometallics*, **2005**, 24, 1556-1562	3.8	99
5	Shape maps and polyhedral interconversion paths in transition metal chemistry. *Coordination Chemistry Reviews*, **2005**, 249, 1693-1708	23.2	727
4	Spin density distribution in transition metal complexes. *Coordination Chemistry Reviews*, **2005**, 249, 2649-2660	23.2	153
3	Mapping the stereochemistry and symmetry of tetracoordinate transition-metal complexes. *Chemistry - A European Journal*, **2004**, 10, 190-207	4.8	152
2	Minimal distortion pathways in polyhedral rearrangements. *Journal of the American Chemical Society*, **2004**, 126, 1755-63	16.4	294
1	Classical molecular interaction potentials: improved setup procedure in molecular dynamics simulations of proteins. *Proteins: Structure, Function and Bioinformatics*, **2001**, 45, 428-37	4.2	79