Jordi Cirera

List of Publications by Year in descending order

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52 papers	5,204 citations	159525 30 h-index	206029 48 g-index
59 all docs	59 docs citations	59 times ranked	6262 citing authors

#	Article	IF	Citations
1	Copper Active Sites in Biology. Chemical Reviews, 2014, 114, 3659-3853.	23.0	1,305
2	Shape maps and polyhedral interconversion paths in transition metal chemistry. Coordination Chemistry Reviews, 2005, 249, 1693-1708.	9.5	889
3	Minimal Distortion Pathways in Polyhedral Rearrangements. Journal of the American Chemical Society, 2004, 126, 1755-1763.	6.6	362
4	Can large magnetic anisotropy and high spin really coexist?. Chemical Communications, 2008, , 52-54.	2.2	215
5	Mapping the Stereochemistry and Symmetry of Tetracoordinate Transition-Metal Complexes. Chemistry - A European Journal, 2004, 10, 190-207.	1.7	175
6	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.	5.2	168
7	Spin density distribution in transition metal complexes. Coordination Chemistry Reviews, 2005, 249, 2649-2660.	9.5	163
8	How to Build Molecules with Large Magnetic Anisotropy. Chemistry - A European Journal, 2009, 15, 4078-4087.	1.7	163
9	Shape and Spin State in Four-Coordinate Transition-Metal Complexes: The Case of the d6 Configuration. Chemistry - A European Journal, 2006, 12, 3162-3167.	1.7	153
10	Accurate Computed Enthalpies of Spin Crossover in Iron and Cobalt Complexes. Journal of Physical Chemistry A, 2009, 113, 10033-10039.	1.1	138
11	Continuous Shape Measures as a Stereochemical Tool in Organometallic Chemistry. Organometallics, 2005, 24, 1556-1562.	1.1	125
12	Benchmarking Density Functional Methods for Calculation of State Energies of First Row Spin-Crossover Molecules. Inorganic Chemistry, 2018, 57, 14097-14105.	1.9	124
13	Theoretical Prediction of Spin-Crossover Temperatures in Ligand-Driven Light-Induced Spin Change Systems. Inorganic Chemistry, 2012, 51, 8194-8201.	1.9	93
14	Stereochemistry and Spin State in Four-Coordinate Transition Metal Compounds. Inorganic Chemistry, 2008, 47, 2871-2889.	1.9	88
15	Classical molecular interaction potentials: Improved setup procedure in molecular dynamics simulations of proteins. Proteins: Structure, Function and Bioinformatics, 2001, 45, 428-437.	1.5	87
16	Ferromagnetic Coupling in Trinuclear, Partial Cubane Cu^{II} Complexes with a Î¼₃â€OH Core: Magnetostructural Correlations. Chemistry - A European Journal, 2007, 13, 9297-9309.	1.7	69
17	Computational assessment on the Tolman cone angles for P-ligands. Dalton Transactions, 2019, 48, 15036-15048.	1.6	62
18	Exchange coupling in CuIIGdIII dinuclear complexes: A theoretical perspective. Comptes Rendus Chimie, 2008, 11, 1227-1234.	0.2	61

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19	How High the Spin? Allowed and Forbidden Spin States in Transition-Metal Chemistry. Angewandte Chemie - International Edition, 2006, 45, 3012-3020.	7.2	53
20	The effects of electronic polarization on water adsorption in metal-organic frameworks: H2O in MIL-53(Cr). Journal of Chemical Physics, 2012, 137, 054704.	1.2	45
21	Quantitative Geometric Descriptions of the Belt Iron Atoms of the Ironâ^'Molybdenum Cofactor of Nitrogenase and Synthetic Iron(II) Model Complexes. Inorganic Chemistry, 2007, 46, 60-71.	1.9	44
22	Molecular Mechanisms of Spin Crossover in the {Fe(pz)[Pt(CN)₄]} Metalâ€"Organic Framework upon Water Adsorption. Journal of the American Chemical Society, 2016, 138, 6123-6126.	6.6	41
23	Chemically crosslinked isoreticular metalâ€"organic frameworks. Chemical Communications, 2013, 49, 3200.	2.2	40
24	An Unprecedented Stimuliâ€Controlled Singleâ€Crystal Reversible Phase Transition of a Metalâ€"Organic Framework and Its Application to a Novel Method of Guest Encapsulation. Advanced Materials, 2018, 30, e1800726.	11.1	39
25	Theoretical Modeling of Spin Crossover in Metalâ€"Organic Frameworks: [Fe(pz)₂Pt(CN)₄] as a Case Study. Inorganic Chemistry, 2014, 53, 11020-11028.	1.9	38
26	Theoretical modeling of two-step spin-crossover transitions in Fe^{II} dinuclear systems. Journal of Materials Chemistry C, 2015, 3, 7954-7961.	2.7	36
27	Structure of the Reduced Copper Active Site in Preprocessed Galactose Oxidase: Ligand Tuning for One-Electron O₂ Activation in Cofactor Biogenesis. Journal of the American Chemical Society, 2016, 138, 13219-13229.	6.6	35
28	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, 16262-16273.	6.6	33
29	Thermal spin crossover in Fe(<scp>ii</scp>) and Fe(<scp>iii</scp>). Accurate spin state energetics at the solid state. Physical Chemistry Chemical Physics, 2020, 22, 4938-4945.	1.3	32
30	Guest effect on spin-crossover frameworks. Reviews in Inorganic Chemistry, 2014, 34, 199-216.	1.8	31
31	Mercurophilic interactions: a theoretical study on the importance of ligands. Physical Chemistry Chemical Physics, 2017, 19, 11645-11654.	1.3	31
32	Electronic Control of Spin-Crossover Properties in Four-Coordinate Bis(formazanate) Iron(II) Complexes. Journal of the American Chemical Society, 2020, 142, 20170-20181.	6.6	27
33	Theoretical Modeling of the Ligand-Tuning Effect over the Transition Temperature in Four-Coordinated Fe^{II} Molecules. Inorganic Chemistry, 2016, 55, 1657-1663.	1.9	26
34	Computational Modeling of Transition Temperatures in Spin-Crossover Systems. Comments on Inorganic Chemistry, 2019, 39, 216-241.	3.0	23
35	Solvation-Guided Design of Fluorescent Probes for Discrimination of Amyloids. Scientific Reports, 2018, 8, 6950.	1.6	21
36	Electronic and Steric Control of the Spin-Crossover Behavior in [(Cp^R)₂Mn] Manganocenes. Inorganic Chemistry, 2018, 57, 702-709.	1.9	20

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37	Microwave assisted synthesis of heterometallic 3dâ€“4f M₄Ln complexes. Dalton Transactions, 2019, 48, 12440-12450.	1.6	19
38	Assessment of the SCAN Functional for Spin-State Energies in Spin-Crossover Systems. Journal of Physical Chemistry A, 2020, 124, 5053-5058.	1.1	18
39	Piano-Stool Ruthenium(II) Complexes with Delayed Cytotoxic Activity: Origin of the Lag Time. Inorganic Chemistry, 2021, 60, 7974-7990.	1.9	16
40	Electronic Structure Modulation in an Exceptionally Stable Nonâ€Heme Nitrosyl Iron(II) Spinâ€Crossover Complex. Chemistry - A European Journal, 2016, 22, 12741-12751.	1.7	15
41	Spinâ€Crossover Properties of an Iron(II) Coordination Nanohoop. Angewandte Chemie - International Edition, 2021, 60, 3515-3518.	7.2	14
42	Stereospinomers of pentacoordinate iron porphyrin complexes: the case of the [Fe(porphyrinato)(CN)]â^' anions. Dalton Transactions, 2013, 42, 7002.	1.6	12
43	Non-Switching 1,2-Dithienylethene-based Diplatinum(II) Complex Showing High Cytotoxicity. Inorganic Chemistry, 2016, 55, 5356-5364.	1.9	10
44	Ferromagnetism in polynuclear systems based on non-linear [MnII2Mn^{III}] building blocks. Inorganic Chemistry Frontiers, 2016, 3, 1272-1279.	3.0	8
45	Accurate calculation of spin-state energy gaps in Fe(iii) spin-crossover systems using density functional methods. Dalton Transactions, 2021, 50, 17635-17642.	1.6	7
46	Controlling the spin-crossover behavior of the [Cr(indenyl)₂] family via ligand functionalization. Dalton Transactions, 2021, 50, 8704-8710.	1.6	5
47	Spin State and Stereochemistry. , 2013, , 441-468.		2
48	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.	1.4	2
49	[Co/Fe(Î±-Alkyl-tpdt)2]xâ^': Alkyl-Substituted Cobalt and Iron Bis-dithiolenethiophenic Complexes. Inorganic Chemistry, 2020, 59, 9261-9269.	1.9	0
50	Spinâ€Crossover Properties of an Iron(II) Coordination Nanohoop. Angewandte Chemie, 2021, 133, 3557-3560.	1.6	0
51	Spin state and stereochemistry in tetracoordinate complexes of dntransition metals. Acta Crystallographica Section A: Foundations and Advances, 2005, 61, c304-c304.	0.3	0
52	Combined use of structural databases, density functional calculations and continuous shape measures: application to four-coordinate transition metal compounds. Acta Crystallographica Section A: Foundations and Advances, 2007, 63, s72-s72.	0.3	0