Joaquim Jornet-Somoza

List of Publications by Year
in descending order

22	878	567281 15	677142 22
papers	citations	h-index	g-index

22	22	22	1091
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Octopus, a computational framework for exploring light-driven phenomena and quantum dynamics in extended and finite systems. Journal of Chemical Physics, 2020, 152, 124119.	3.0	210
2	Synthesis, Structure, and Magnetic Properties of an Antiferromagnetic Spin-Ladder Complex:Â Bis(2,3-dimethylpyridinium) Tetrabromocuprate. Journal of the American Chemical Society, 2007, 129, 952-959.	13.7	121
3	Calculation of microscopic exchange interactions and modelling of macroscopic magnetic properties in molecule-based magnets. Chemical Society Reviews, 2011, 40, 3182.	38.1	77
4	Origin of the Magnetic Bistability in Molecule-Based Magnets: A First-Principles Bottom-Up Study of the TTTA Crystal. Journal of the American Chemical Society, 2010, 132, 17817-17830.	13.7	61
5	Direct versus Mediated Through-Space Magnetic Interactions: A First Principles, Bottom-Up Reinvestigation of the Magnetism of the Pyridyl-Verdazyl:Hydroquinone Molecular Co-Crystal. Chemistry - A European Journal, 2006, 12, 3995-4005.	3.3	59
6	Synthesis, Structure, and Magnetic Behavior of Bis(2-amino-5-fluoropyridinium) Tetrachlorocuprate(II). Inorganic Chemistry, 2007, 46, 11254-11265.	4.0	57
7	Insights into colour-tuning of chlorophyll optical response in green plants. Physical Chemistry Chemical Physics, 2015, 17, 26599-26606.	2.8	46
8	First-Principles Bottom-Up Study of 1D to 3D Magnetic Transformation in the Copper Pyrazine Dinitrate S = 1/2 Antiferromagnetic Crystal. Inorganic Chemistry, 2010, 49, 1750-1760.	4.0	33
9	Synthesis, Structure, Magnetic Behavior, and Theoretical Analysis of Diazine-Bridged Magnetic Ladders: Cu(quinoxoline)X2 and Cu(2,3-dimethylpyrazine)X2 (X = Cl, Br). Inorganic Chemistry, 2012, 51, 6315-6325.	4.0	27
10	Covalent Câ€“N Bond Formation through a Surface Catalyzed Thermal Cyclodehydrogenation. Journal of the American Chemical Society, 2020, 142, 3696-3700.	13.7	27
11	A generalised 17-state vibronic-coupling Hamiltonian model for ethylene. Journal of Chemical Physics, 2012, 137, 084304.	3.0	25
12	Real-Time Propagation TDDFT and Density Analysis for Exciton Coupling Calculations in Large Systems. Journal of Chemical Theory and Computation, 2019, 15, 3743-3754.	5.3	24
13	Dividing the Spoils: Role of Pyrazine Ligands and Perchlorate Counterions in the Magnetic Properties of Bis(pyrazine)diperchloratecopper(II), [Cu(pz)₂](ClO₄)₂. Inorganic Chemistry, 2013, 52, 12923-12932.	4.0	22
14	On the existence of temperature induced changes in the magnetic topology of crystals that show no first-order crystallographic phase transitions. Polyhedron, 2009, 28, 1965-1971.	2.2	17
15	Vertical transition energies vs. absorption maxima: Illustration with the UV absorption spectrum of ethylene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 119, 52-58.	3.9	17
16	The Magnetism of (5MAP)₂CuBr₄ [5MAP = 5-Methyl-2-aminopyridinium]: A Quasi-2D or a 3D Magnetic System?. Inorganic Chemistry, 2010, 49, 8017-8024.	4.0	13
17	The origin of the bistability in the thiazyl radical 1,3,5-trithia-2,4,6-triazapentalenyl (TTTA): A first principles bottom-up investigation of the magnetic properties of its high temperature polymorph. Polyhedron, 2009, 28, 1614-1619.	2.2	10
18	Revising the common understanding of metamagnetism in the molecule-based bisdithiazolyl BDTMe compound. Physical Chemistry Chemical Physics, 2019, 21, 12184-12191.	2.8	8

#	Article	IF	Citations
19	A first-principles bottom-up study of the magnetic interaction mechanism in the bulk ferromagnet p-O2N-C6F4-CNSSN. Inorganica Chimica Acta, 2008, 361, 3586-3592.	2.4	7
20	Pitfalls on evaluating pair exchange interactions for modelling molecule-based magnetism. Journal of Materials Chemistry C, 2021, 9, 10647-10660.	5.5	7
21	A Definition of the Magnetic Transition Temperature Using Valence Bond Theory. Journal of Physical Chemistry A, 2018, 122, 2168-2177.	2.5	5
22	Disentangling the magnetic dimensionality of an alleged magnetically isolated cuprate spin-ladder CuHpCl system: a long-lasting issue. Dalton Transactions, 2021, 50, 1754-1765.	3.3	5