Jordi Ribas

List of Publications by Year in descending order

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97 papers	3,052 citations	136740 32 h-index	182168 51 g-index
106 all docs	106 docs citations	106 times ranked	3255 citing authors

#	Article	IF	Citations
1	Controlling Chemical Reactivity with Optimally Oriented Electric Fields: A Generalization of the Newton Trajectory Method. Journal of Chemical Theory and Computation, 2022, 18, 935-952.	2.3	6
2	Electronic structure and magnetic coupling in selenium substituted pyridine-bridged bisdithiazolyl multifunctional molecular materials. Physical Chemistry Chemical Physics, 2022, 24, 12196-12207.	1.3	2
3	2D Hexagonal Covalent Organic Radical Frameworks as Tunable Correlated Electron Systems. Advanced Functional Materials, 2021, 31, 2004584.	7.8	14
4	Structural, ferroelectric, and optical properties of <scp>Bi³⁺</scp> doped <scp>YFeO₃</scp>: A firstâ€principles study. International Journal of Quantum Chemistry, 2021, 121, e26551.	1.0	4
5	Refined metadynamics through canonical sampling using timeâ€invariant bias potential: A study of polyalcohol dehydration in hot acidic solutions. Journal of Computational Chemistry, 2021, 42, 156-165.	1.5	5
6	Twistable dipolar aryl rings as electric field actuated conformational molecular switches. Physical Chemistry Chemical Physics, 2021, 23, 3844-3855.	1.3	9
7	Barnes Update Applied in the Gaussâ€“Newton Method: An Improved Algorithm to Locate Bond Breaking Points. Journal of Chemical Theory and Computation, 2021, 17, 996-1007.	2.3	6
8	Insights into the magnetism and phase transitions of organic radical-based materials. Journal of Materials Chemistry C, 2021, 9, 10624-10646.	2.7	27
9	Pitfalls on evaluating pair exchange interactions for modelling molecule-based magnetism. Journal of Materials Chemistry C, 2021, 9, 10647-10660.	2.7	7
10	Controlling pairing of Ï€-conjugated electrons in 2D covalent organic radical frameworks via in-plane strain. Nature Communications, 2021, 12, 1705.	5.8	18
11	Low temperature structures and magnetic interactions in the organic-based ferromagnetic and metamagnetic polymorphs of decamethylferrocenium 7,7,8,8-tetracyano-p-quinodimethanide, [FeCp*2]Ë™+[TCNQ]Ë™â^'. Dalton Transactions, 2021, 50, 11228-11242.	1.6	6
12	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
13	First-principles study of the coexisting ferroelectric and ferromagnetic properties of the La0.75Bi0.25CrO3 compound. Computational Materials Science, 2020, 171, 109262.	1.4	6
14	Structural, electronic and ferroelectric properties of Zn93.75M6.25O (MÂ=ÂSr, Ba): first-principles calculations. Scripta Materialia, 2020, 187, 8-12.	2.6	1
15	Two different mechanisms of stabilization of regular Ï€-stacks of radicals in switchable dithiazolyl-based materials. Journal of Materials Chemistry C, 2020, 8, 5437-5448.	2.7	7
16	Effect of La3+/Sr2+ ordering on the magnetic properties of La2/3Sr1/3MnO3 by first principles calculations. Computational Materials Science, 2020, 177, 109575.	1.4	2
17	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
18	Interplay between the Gentlest Ascent Dynamics Method and Conjugate Directions to Locate Transition States. Journal of Chemical Theory and Computation, 2019, 15, 5426-5439.	2.3	3

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19	Understanding Competition of Polyalcohol Dehydration Reactions in Hot Water. Journal of Physical Chemistry B, 2019, 123, 1662-1671.	1.2	4
20	Reorganization of Intermolecular Interactions in the Polymorphic Phase Transition of a Prototypical Dithiazolyl-Based Bistable Material. Crystal Growth and Design, 2019, 19, 2329-2339.	1.4	7
21	Selective Nanomechanics of Aromatic versus Aliphatic Thiolates on Gold Surfaces. Physical Review Letters, 2019, 122, 086801.	2.9	1
22	Toward a theory of mechanochemistry: Simple models from the very beginnings. International Journal of Quantum Chemistry, 2018, 118, e25775.	1.0	18
23	The magnetic fingerprint of dithiazolyl-based molecule magnets. Physical Chemistry Chemical Physics, 2018, 20, 20406-20416.	1.3	16
24	Bistability in Organic Magnetic Materials: A Comparative Study of the Key Differences between Hysteretic and Nonâ€hysteretic Spin Transitions in Dithiazolyl Radicals. Chemistry - A European Journal, 2017, 23, 3479-3489.	1.7	26
25	Ferromagnetic Exchange in Bichloride Bridged Cu(II) Chains: Magnetostructural Correlations between Ordered and Disordered Systems. Inorganic Chemistry, 2017, 56, 5441-5454.	1.9	10
26	Molecules Designed to Contain Two Weakly Coupled Spins with a Photoswitchable Spacer. Chemistry - A European Journal, 2017, 23, 13648-13659.	1.7	22
27	Lattice-Solvent Effects in the Spin-Crossover of an Fe(II)-Based Material. The Key Role of Intermolecular Interactions between Solvent Molecules. Inorganic Chemistry, 2017, 56, 4474-4483.	1.9	36
28	Analysis of the Acting Forces in a Theory of Catalysis and Mechanochemistry. Journal of Physical Chemistry A, 2017, 121, 2820-2838.	1.1	24
29	Origin of Bistability in the Butylâ€Substituted Spirobiphenalenylâ€Based Neutral Radical Material. Chemistry - A European Journal, 2017, 23, 7772-7784.	1.7	10
30	An algorithm to locate optimal bond breaking points on a potential energy surface for applications in mechanochemistry and catalysis. Journal of Chemical Physics, 2017, 147, 152710.	1.2	22
31	Unexpected mechanochemical complexity in the mechanistic scenarios of disulfide bond reduction in alkaline solution. Nature Chemistry, 2017, 9, 164-170.	6.6	60
32	Disclosing the Ligand- and Solvent-Induced Changes on the Spin Transition and Optical Properties of Fe(II)-Indazolylpyridine Complexes. Magnetochemistry, 2016, 2, 6.	1.0	10
33	On the zerothâ€order hamiltonian for <scp>CASPT</scp>2 calculations of spin crossover compounds. Journal of Computational Chemistry, 2016, 37, 947-953.	1.5	36
34	Forceâ€Induced Reversal of Î²â€Eliminations: Stressed Disulfide Bonds in Alkaline Solution. Angewandte Chemie - International Edition, 2016, 55, 1304-1308.	7.2	16
35	Formation of Long, Multicenter Ï€â€[TCNE]₂^{2â^’} Dimers in Solution: Solvation and Stability Assessed through Molecular Dynamics Simulations. Chemistry - A European Journal, 2016, 22, 17037-17046.	1.7	7
36	The reaction mechanism of polyalcohol dehydration in hot pressurized water. Physical Chemistry Chemical Physics, 2016, 18, 32438-32447.	1.3	8

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37	Forceâ€Induced Reversal of Î²â€Eliminations: Stressed Disulfide Bonds in Alkaline Solution. Angewandte Chemie, 2016, 128, 1326-1330.	1.6	3
38	Towards an accurate and computationally-efficient modelling of Fe(<scp>ii</scp>)-based spin crossover materials. Physical Chemistry Chemical Physics, 2015, 17, 16306-16314.	1.3	53
39	Electronic Excitation Energies in Dimers between Radical Ions Presenting Long, Multicenter Bonding. Journal of Chemical Theory and Computation, 2015, 11, 2651-2660.	2.3	6
40	Nanomechanics of Bidentate Thiolate Ligands on Gold Surfaces. Physical Review Letters, 2015, 114, 075501.	2.9	8
41	Unravelling the Key Driving Forces of the Spin Transition in Ï€-Dimers of Spiro-biphenalenyl-Based Radicals. Journal of the American Chemical Society, 2015, 137, 12843-12855.	6.6	20
42	New coordination features; a bridging pyridine and the forced shortest non-covalent distance between two CO₃^{2â^'} species. Chemical Science, 2015, 6, 123-131.	3.7	20
43	Dynamical effects on the magnetic properties of dithiazolyl bistable materials. Chemical Science, 2015, 6, 2371-2381.	3.7	34
44	Towards the tailored design of benzotriazinyl-based organic radicals displaying a spin transition. Chemical Communications, 2015, 51, 15776-15779.	2.2	16
45	The Effect of Tensile Stress on the Conformational Free Energy Landscape of Disulfide Bonds. PLoS ONE, 2014, 9, e108812.	1.1	14
46	Elucidating the 2D Magnetic Topology of the â€˜Metalâ€“Radicalâ€™ TTTAâ‹…Cu(hfac)₂ System. Chemistry - A European Journal, 2014, 20, 7083-7090.	1.7	16
47	On the Importance of Thermal Effects and Crystalline Disorder in the Magnetism of Benzotriazinylâ€Derived Organic Radicals. Chemistry - an Asian Journal, 2014, 9, 3612-3622.	1.7	14
48	S=1/2 Oneâ€Dimensional Randomâ€Exchange Ferromagnetic Zigzag Ladder, Which Exhibits Competing Interactions in a Critical Regime. Chemistry - A European Journal, 2014, 20, 8355-8362.	1.7	15
49	Insights into the crystal-packing effects on the spin crossover of [Fe^{II}(1-bpp)]²⁺-based materials. Physical Chemistry Chemical Physics, 2014, 16, 27012-27024.	1.3	57
50	Structural and Magnetic Diversity Based on Different Imidazolate Linkers in Cu(II)-Azido Coordination Compounds. Inorganic Chemistry, 2014, 53, 11991-12001.	1.9	13
51	Assessing the Performance of CASPT2 and DFT Methods for the Description of Long, Multicenter Bonding in Dimers between Radical Ions. Journal of Chemical Theory and Computation, 2014, 10, 650-658.	2.3	29
52	The key role of vibrational entropy in the phase transitions of dithiazolyl-based bistable magnetic materials. Nature Communications, 2014, 5, 4411.	5.8	55
53	Linear or Cyclic Clusters of Cu(II) with a Hierarchical Relationship. Inorganic Chemistry, 2014, 53, 3290-3297.	1.9	16
54	Two isosceles coordination [Ni3] triangles strongly interacting via hydrogen bonds. Polyhedron, 2013, 52, 1369-1374.	1.0	13

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55	The Janus-faced role of external forces in mechanochemical disulfide bond cleavage. Nature Chemistry, 2013, 5, 685-691.	6.6	82
56	Unraveling the Role of Water in the Stereoselective Step of Aqueous Prolineâ€Catalyzed Aldol Reactions. Chemistry - A European Journal, 2012, 18, 15868-15874.	1.7	19
57	A Heterometallic (Ni^{II}â€“Cu^{II}) Decanuclear Cluster Containing Two Distorted Cubane-like Pentanuclear Cores: Synthesis, Structure, and Magnetic Properties. Inorganic Chemistry, 2012, 51, 6440-6442.	1.9	32
58	Tracing the Sources of the Different Magnetic Behavior in the Two Phases of the Bistable (BDTA)₂[Co(mnt)₂] Compound. Inorganic Chemistry, 2012, 51, 8646-8648.	1.9	12
59	Covalent Mechanochemistry: Theoretical Concepts and Computational Tools with Applications to Molecular Nanomechanics. Chemical Reviews, 2012, 112, 5412-5487.	23.0	346
60	A 3D Cu^{II} Coordination Framework with Î¼₄-/Î¼₂-Oxalato Anions and a Bent Dipyridyl Coligand: Unique Zeolite-Type NiP₂ Topological Network and Magnetic Properties. Inorganic Chemistry, 2011, 50, 6850-6852.	1.9	31
61	On the role of polymer chains in transducing external mechanical forces to benzocyclobutene mechanophores. Journal of Materials Chemistry, 2011, 21, 8309.	6.7	55
62	Forceâ€Transformed Freeâ€Energy Surfaces and Trajectoryâ€Shooting Simulations Reveal the Mechanoâ€Stereochemistry of Cyclopropane Ringâ€Opening Reactions. Angewandte Chemie - International Edition, 2011, 50, 7105-7108.	7.2	44
63	Revealing the Magnetostructural Dynamics of [2Fe-2S] Ferredoxins from Reduced-Dimensionality Analysis of Antiferromagnetic Exchange Coupling Fluctuations. Journal of Physical Chemistry B, 2010, 114, 11612-11619.	1.2	14
64	Magnetostructural Dynamics from Hubbard-U Corrected Spin-Projection: [2Feâ^'2S] Complex in Ferredoxin. Journal of Chemical Theory and Computation, 2010, 6, 569-575.	2.3	19
65	Mechanochemical Transduction of Externally Applied Forces to Mechanophores. Journal of the American Chemical Society, 2010, 132, 10609-10614.	6.6	98
66	Hydrogen bond assisted co-crystallization of a bimetallic Mn^{III}₂Ni^{II}₂cluster and a Ni^{II}₂cluster unit: synthesis, structure, spectroscopy and magnetism. Dalton Transactions, 2010, 39, 4986-4990.	1.6	16
67	Designed Topology and Siteâ€Selective Metal Composition in Tetranuclear [MMâ€²â‹…â‹…â‹…Mâ€²M] Linear Complexes. Chemistry - A European Journal, 2009, 15, 11235-11243.	1.7	41
68	Unravelling the Mechanism of Forceâ€Induced Ringâ€Opening of Benzocyclobutenes. Chemistry - A European Journal, 2009, 15, 13331-13335.	1.7	47
69	Understanding Covalent Mechanochemistry. Angewandte Chemie - International Edition, 2009, 48, 4190-4193.	7.2	231
70	Structure and Magnetic Interactions in the Organic-Based Ferromagnet Decamethylferrocenium Tetracyanoethenide, [FeCp*2]â€¢+[TCNE]â€¢â^'. Inorganic Chemistry, 2009, 48, 3296-3307.	1.9	34
71	Strong through-space two-halide magnetic exchange of â^'234 K in (2,5-dimethylpyrazine)copper(ii) bromide. Chemical Communications, 2009, , 1359.	2.2	35
72	Study of the magnetic exchange within the cluster polymer [NaCu6(gly)8(ClO4)3(H2O)]n(ClO4)2n. Inorganica Chimica Acta, 2008, 361, 3919-3925.	1.2	10

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73	A Versatile Series of Nickel(II) Complexes Derived from Tetradentate Imine/Pyridyl Ligands and Various Pseudohalides: Azide and Cyanate Compared. Inorganic Chemistry, 2008, 47, 4109-4117.	1.9	66
74	A novel [CuII4] cluster from the assembly of two [CuII2L]+units by a central Âµ4-1,1,2,2 perchlorate ligand. Dalton Transactions, 2008, , 861-864.	1.6	31
75	Self-Assembly of an Azido-Bridged [Ni^{II}₆] Cluster Featuring Four Fused Defective Cubanes. Inorganic Chemistry, 2008, 47, 3465-3467.	1.9	71
76	The mechanism for the reversible oxygen addition to heme. A theoretical CASPT2 study. Chemical Communications, 2007, , 3160.	2.2	40
77	Two Cu2and Zn2Metallamacrocycles Featuring a Novel Extended Ï€-Conjugated Carbazole Bridge. Inorganic Chemistry, 2007, 46, 2947-2949.	1.9	28
78	Control of Two-Electron Four-Center (2e-/4c) Câ^'C Bond Formation Observed for Tetracyanoethenide Dimerization, [TCNE]22-. Inorganic Chemistry, 2007, 46, 103-107.	1.9	17
79	Preparation and Structure of Three Solvatomorphs of the Polymer [Co(dbm)₂(4ptz)]_n:â€‰ Spin Canting Depending on the Supramolecular Organization. Inorganic Chemistry, 2007, 46, 7154-7162.	1.9	50
80	Structures with Tunable Strong Ferromagnetic Coupling: from Unordered (1D) to Ordered (Discrete). Chemistry - A European Journal, 2007, 13, 9924-9930.	1.7	87
81	Analysis of the magneto-structural correlations in the meso-tetraphenylporphyrinatomanganese(iii) tetracyanoethenide family of molecule-based magnets. Journal of Materials Chemistry, 2006, 16, 2600-2611.	6.7	33
82	Toward the Control of the Magnetic Anisotropy of FeIICubes:Â A DFT Study. Journal of the American Chemical Society, 2006, 128, 9497-9505.	6.6	47
83	Structural and Magnetic Properties of a Complete Halide Series of NiII Complexes with a Pyridine-Containing 14-Membered Macrocycle. Inorganic Chemistry, 2006, 45, 7621-7627.	1.9	23
84	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.	1.7	59
85	Generalized Stone-Wales transformation as the possible origin of ferromagnetism in polymeric C60: A density-functional theory study. Journal of Chemical Physics, 2006, 125, 174312.	1.2	4
86	Ferromagnetism in pressed polymerizedC60solids induced byC60cage vacancies: A density-functional study. Physical Review B, 2006, 73, .	1.1	9
87	Density-functional study of two Fe4-based single-molecule magnets. Journal of Chemical Physics, 2005, 123, 044303.	1.2	34
88	Substituted m-phenylene bridges as strong ferromagnetic couplers for Cuiiâ€“bridgeâ€“Cuii magnetic interactions: new perspectives. Chemical Communications, 2005, , 5172.	2.2	65
89	Broken Inter-C60Bonds as the Cause of Magnetism in Polymeric C60:Â A Density Functional Study Using C60Dimers. Journal of Physical Chemistry A, 2005, 109, 4979-4982.	1.1	2
90	A First-Principles Analysis of the Magnetism of CuII Polynuclear Coordination Complexes: the Case of [Cu4(bpy)4(aspartate)2(H2O)3](ClO4)4â€¢2.5H2O. Molecules, 2004, 9, 757-770.	1.7	12

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91	The Origin of the Magnetic Moments in Compressed Crystals of Polymeric C60. Angewandte Chemie - International Edition, 2004, 43, 577-580.	7.2	17
92	The Origin of the Magnetic Moments in Compressed Crystals of Polymeric C60.. ChemInform, 2004, 35, no.	0.1	0
93	Evaluation of the capability of C60-fullerene to act as a magnetic coupling unit. Journal of Physics and Chemistry of Solids, 2004, 65, 787-791.	1.9	17
94	Self-Assembly of CuIIand NiII[2 Ã— 2] Grid Complexes and a Binuclear CuIIComplex with a New Semiflexible Substituted Pyrazine Ligand:Â Multiple Anion Encapsulation and Magnetic Properties. Inorganic Chemistry, 2004, 43, 1021-1030.	1.9	64
95	A new tetrameric CuIIcluster with square topology exhibiting ferro- and antiferromagnetic magnetic pathways : which is which?. Chemical Communications, 2004, , 1102-1103.	2.2	38
96	Theoretical Study of Alkyl-Ï€ and Aryl-Ï€ Interactions. Reconciling Theory and Experiment. Journal of Organic Chemistry, 2002, 67, 7057-7065.	1.7	119
97	Serving science through publishing. , 0, 1, 1.		1