MercÃ¨ Deumal

List of Publications by Year
in descending order

66 papers	1,513 citations	331538 21 h-index	330025 37 g-index
72 all docs	72 docs citations	72 times ranked	1009 citing authors

#	ARTICLE	IF	CITATIONS
1	Approaching the isotropic spin-ladder regime: structure and magnetism of all-pyrazine-bridged copper(<scp>ii</scp>)-based antiferromagnetic ladders. Dalton Transactions, 2022, 51, 4653-4667.	1.6	2
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	Disentangling the magnetic dimensionality of an alleged magnetically isolated cuprate spin-ladder CuHpCl system: a long-lasting issue. Dalton Transactions, 2021, 50, 1754-1765.	1.6	5
5	Insights into the magnetism and phase transitions of organic radical-based materials. Journal of Materials Chemistry C, 2021, 9, 10624-10646.	2.7	27
6	Pitfalls on evaluating pair exchange interactions for modelling molecule-based magnetism. Journal of Materials Chemistry C, 2021, 9, 10647-10660.	2.7	7
7	Controlling pairing of Ï€-conjugated electrons in 2D covalent organic radical frameworks via in-plane strain. Nature Communications, 2021, 12, 1705.	5.8	18
8	Assessing Cu2L2X4 dimeric moieties as ferromagnetic building blocks in double halide-bridged polymers (XÂ=ÂClâ^', Brâ^' and LÂ=Âbenzamide). An experimental and computational study. Polyhedron, 2020, 185, 114603.	1.0	2
9	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
10	Revisiting the Role of Hydrogen Bonding in the Strong Dimer Superexchange of a 2D Copper(II) Halide Honeycomb-Like Lattice: Structural and Magnetic Study. Inorganic Chemistry, 2020, 59, 6319-6331.	1.9	4
11	Revising the common understanding of metamagnetism in the molecule-based bisdithiazolyl BDTMe compound. Physical Chemistry Chemical Physics, 2019, 21, 12184-12191.	1.3	8
12	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
13	A Definition of the Magnetic Transition Temperature Using Valence Bond Theory. Journal of Physical Chemistry A, 2018, 122, 2168-2177.	1.1	5
14	The magnetic fingerprint of dithiazolyl-based molecule magnets. Physical Chemistry Chemical Physics, 2018, 20, 20406-20416.	1.3	16
15	The quest for rationalizing the magnetism in purely organic semiquinone-bridged bisdithiazolyl molecular magnets. Physical Chemistry Chemical Physics, 2016, 18, 20738-20749.	1.3	10
16	The origin of the antiferromagnetic behaviour of the charge-transfer compound (HMTTF)[Ni(mnt)₂]. Dalton Transactions, 2015, 44, 608-614.	1.6	5
17	Dynamical effects on the magnetic properties of dithiazolyl bistable materials. Chemical Science, 2015, 6, 2371-2381.	3.7	34
18	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

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19	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
20	The key role of vibrational entropy in the phase transitions of dithiazolyl-based bistable magnetic materials. Nature Communications, 2014, 5, 4411.	5.8	55
21	A theoretical analysis of the magnetic properties of the low-dimensional copper(II)X2(2-X-3-methylpyridine)2 (X = Cl and Br) complexes. Highlights in Theoretical Chemistry, 2014, , 219-230.	0.0	0
22	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.	1.9	22
23	A theoretical analysis of the magnetic properties of the low-dimensional copper(II)X2(2-X-3-methylpyridine)2 (XÂ=ÂCl and Br) complexes. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	4
24	A theoretical analysis of the magnetic properties of the low dimensional bis(2-chloropyrazine)dichlorocopper(II) molecule-based magnet. Polyhedron, 2013, 64, 163-171.	1.0	2
25	Assigning the dimensionality in low-dimensional materials: A rigorous study of the dimensionality of (2,5-dimethylpyrazine)CuCl2. Polyhedron, 2013, 52, 699-705.	1.0	6
26	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.	1.9	27
27	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
28	Calculation of microscopic exchange interactions and modelling of macroscopic magnetic properties in molecule-based magnets. Chemical Society Reviews, 2011, 40, 3182.	18.7	77
29	Studying the Origin of the Antiferromagnetic to Spinâ€Canting Transition in the Î²â€pâ€NCC₆F₄CNSSN[.]Molecular Magnet. Chemistry - A European Journal, 2010, 16, 2741-2750.	1.7	51
30	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.	1.9	33
31	The Magnetism of (5MAP)₂CuBr₄ [5MAP = 5-Methyl-2-aminopyridinium]: A Quasi-2D or a 3D Magnetic System?. Inorganic Chemistry, 2010, 49, 8017-8024.	1.9	13
32	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.	6.6	61
33	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.	1.0	10
34	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.	1.0	17
35	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.	1.2	7
36	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.	6.6	121

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37	Synthesis, Structure, and Magnetic Behavior of Bis(2-amino-5-fluoropyridinium) Tetrachlorocuprate(II). Inorganic Chemistry, 2007, 46, 11254-11265.	1.9	57
38	A theoretical study of the magnetism of the Î±-p-cyano-tetrafluorophenyl-dithiadiazolyl radical using a first principles bottom-up procedure. Polyhedron, 2007, 26, 1949-1958.	1.0	32
39	Theoretical study of the magnetism in molecular crystals using a first-principles bottom-up methodol. Progress in Theoretical Chemistry and Physics, 2007, , 271-289.	0.2	15
40	Bulk ferromagnetism in nitronyl nitroxide crystals: a first principles bottom-up comparative study of four bulk nitronyl nitroxide ferromagnets (KAXHAS, YOMYII, LICMIT and YUJNEW). Molecular Physics, 2006, 104, 857-873.	0.8	20
41	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
42	Quantitative analysis of the magnetism of the meta-(methoxy)phenyl nitronyl nitroxide crystal: A bottomâ€“up analysis of a crystal presenting competing ferro and antiferromagnetic interactions. Polyhedron, 2005, 24, 2368-2376.	1.0	5
43	The Mechanism of Magnetic Interaction in Spin-Ladder Molecular Magnets: A First-Principles, Bottom-Up, Theoretical Study of the Magnetism in the Two-Legged Spin-Ladder Bis(2-amino-5-nitropyridinium) Tetrabromocuprate Monohydrate. European Journal of Inorganic Chemistry, 2005, 2005, 4697-4706.	1.0	35
44	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
45	The Mechanism of Magnetic Interactions in the Bulk Ferromagnetpara-(Methylthio)Phenyl Nitronyl Nitroxide (YUJNEW): A First Principles, Bottom-Up, Theoretical Study. Chemistry - A European Journal, 2004, 10, 6422-6432.	1.7	37
46	Theoretical Study of the Electronic Structure and Magnetic Interactions in Purely Organic Nitronyl Nitroxide Crystals. ChemInform, 2003, 34, no.	0.1	0
47	The mechanism of the magnetic interaction in the Î² phase of the p -(nitro)phenyl nitronyl nitroxide (KAXHAS). A bottom-up study using only ab initio data. Polyhedron, 2003, 22, 1935-1944.	1.0	23
48	Through space magnetic exchange in tetrabromocuprates: theoretical considerations. Polyhedron, 2003, 22, 2235-2239.	1.0	15
49	Magnetic Properties of Organic Molecular Crystals via an Algebraic Heisenberg Hamiltonian. Applications to WILVIW, TOLKEK, and KAXHAS Nitronyl Nitroxide Crystals. Journal of Physical Chemistry A, 2002, 106, 1299-1315.	1.1	87
50	A general study of the spin population of Î±-nitronyl nitroxide radicals: radicals with crystals presenting dominant ferro or antiferromagnetic behavior. Synthetic Metals, 2001, 122, 477-483.	2.1	15
51	The Mechanism of the Through-Space Magnetic Interactions in Purely Organic Molecular Magnets. , 2001, , 33-60.		30
52	The microscopic basis of the intermolecular magnetism. An ab initio study on molecular crystals. Computational and Theoretical Chemistry, 2000, 506, 287-296.	1.5	6
53	Does the McConnell-I Model Really Work? An ab Initio Study of the Magnetic Character of Some Intermolecular Contacts. Molecular Crystals and Liquid Crystals, 1999, 335, 603-612.	0.3	8
54	Structure-Magnetism Relationships inÎ±-Nitronyl Nitroxide Radicals. Chemistry - A European Journal, 1999, 5, 1631-1642.	1.7	103

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55	Architecture of purely organic molecular magnets: Crystal packing rationalization of some Î±-nitronyl nitroxides using the crystal packing functional group analysis. Synthetic Metals, 1999, 103, 2283-2286.	2.1	6
56	Structureâ€“Magnetism Relationships in Î±-Nitronyl Nitroxide Radicals. , 1999, 5, 1631.		1
57	Crystal Engineering of Purely Organic Molecular Magnets: What can AB Initio Computations Tell Us?. , 1999, , 105-125.		0
58	Structure-Magnetism Relationships in Î±-Nitronyl Nitroxide Radicals: Pitfalls and Lessons to be Learned. Advanced Materials, 1998, 10, 1461-1466.	11.1	48
59	Product Distributions from Molecular Mechanicsâ^'Valence Bond Dynamics:Â Modeling Photochemical [4 + 4] Cycloadditions. Journal of Organic Chemistry, 1998, 63, 4594-4600.	1.7	14
60	On the Validity of the McConnell-I Model of Ferromagnetic Interactions:â€‰ The [2.2]Paracyclophane Example. Journal of Physical Chemistry A, 1998, 102, 8404-8412.	1.1	68
61	Structureâ€“Magnetism Relationships in Î±-Nitronyl Nitroxide Radicals: Pitfalls and Lessons to be Learned. Advanced Materials, 1998, 10, 1461-1466.	11.1	1
62	A Theoretical Analysis of the Packing and Polymorphism of the 2-Hydro Nttronyl Nitroxide Crystal. Molecular Crystals and Liquid Crystals, 1997, 305, 129-141.	0.3	7
63	Modeling Photochemical [4 + 4] Cycloadditions:Â Conical Intersections Located with CASSCF for Butadiene + Butadiene. Journal of the American Chemical Society, 1997, 119, 709-718.	6.6	38
64	Theoretical Analysis of the Packing and Polimorphism of Molecular Crystals Using Quantum Mechanical Methods: The Packing of the 2-Hydro Nitronyl Nitroxide. Molecular Crystals and Liquid Crystals, 1997, 305, 143-156.	0.3	18
65	Theoretical analysis of the crystal packing of nitronyl nitroxide radicals: the packing of the Î±-2-hydro nitronyl nitroxide radical. Chemical Physics Letters, 1997, 265, 190-199.	1.2	25
66	Theoretical Study of the Electronic Structure and Magnetic Interactions in Purely Organic Nitronyl Nitroxide Crystals. , 0, , 65-117.		1