Sergi Vela

List of Publications by Year
in descending order

54 papers	979 citations	393982 19 h-index	476904 29 g-index
61 all docs	61 docs citations	61 times ranked	1293 citing authors

#	Article	IF	Citations
1	Heteroatom oxidation controls singletâ€"triplet energy splitting in singlet fission building blocks. Chemical Communications, 2022, 58, 1338-1341.	2.2	6
2	Donorâ€"Acceptorâ€"Donor â€œHot Excitonâ€•Triads for High Reverse Intersystem Crossing in OLEDs. Advanced Optical Materials, 2022, 10, .	3.6	7
3	Insights into the magnetism and phase transitions of organic radical-based materials. Journal of Materials Chemistry C, 2021, 9, 10624-10646.	2.7	27
4	Pitfalls on evaluating pair exchange interactions for modelling molecule-based magnetism. Journal of Materials Chemistry C, 2021, 9, 10647-10660.	2.7	7
5	Identifying the Trade-off between Intramolecular Singlet Fission Requirements in Donorâ€"Acceptor Copolymers. Chemistry of Materials, 2021, 33, 2567-2575.	3.2	14
6	Learning the Exciton Properties of Azo-dyes. Journal of Physical Chemistry Letters, 2021, 12, 5957-5962.	2.1	4
7	Tuning the Thermal Stability and Photoisomerization of Azoheteroarenes through Macrocycle Strain**. Chemistry - A European Journal, 2021, 27, 419-426.	1.7	12
8	Bi-stable spin-crossover in charge-neutral [Fe(R-ptp)₂] (ptp =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 467 Td (2-(1<i>H</i>-p 1022-1031.	1.6	16
9	The Photoisomerization Pathway(s) of Pushâ€"Pull Phenylazoheteroarenes**. Chemistry - A European Journal, 2020, 26, 14724-14729.	1.7	6
10	Designing Singlet Fission Candidates from Donorâ€"Acceptor Copolymers. Chemistry of Materials, 2020, 32, 6515-6524.	3.2	27
11	Extremely well isolated two-dimensional spin- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mfrac><mml:mn>1</mml:mn><mml:mn>2</mml:mn></mml:mfrac></m antiferromagnetic Heisenberg layers with a small exchange coupling in the molecular-based magnet CuPOF. Physical Review B, 2020, 102, .	1.1	8
12	Reversible Magnetic Transition in a Bench-Stable Radical Cation Triggered by Structural Transition in the Magnetically Silent Counteranion. Crystal Growth and Design, 2020, 20, 6296-6301.	1.4	10
13	Structure:function relationships for thermal and light-induced spin-crossover in isomorphous molecular materials. Journal of Materials Chemistry C, 2020, 8, 8420-8429.	2.7	11
14	Assessing Cu2L2X4 dimeric moieties as ferromagnetic building blocks in double halide-bridged polymers (XÂ=ÂClâˆ', Brâˆ' and LÂ=Âbenzamide). An experimental and computational study. Polyhedron, 2020, 185, 114603.	1.0	2
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	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
17	Exploring chemical space in the search for improved azoheteroarene-based photoswitches. Physical Chemistry Chemical Physics, 2019, 21, 20782-20790.	1.3	10
18	Deciphering crystal packing effects in the spin crossover of six [Fe^{II}(2-pic)₃]Cl₂solvatomorphs. Dalton Transactions, 2019, 48, 1237-1245.	1.6	18

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19	Revising the common understanding of metamagnetism in the molecule-based bisdithiazolyl BDTMe compound. Physical Chemistry Chemical Physics, 2019, 21, 12184-12191.	1.3	8
20	Bi-stable spin-crossover characteristics of a highly distorted [Fe(1-BPP-COOC₂H₅)₂](ClO₄)₂Â·CH₃CN complex. Dalton Transactions, 2019, 48, 3825-3830.	1.6	27
21	Controlling the crystallinity and crystalline orientation of â€œshuttlecockâ€• naphthalocyanine films for near-infrared optoelectronic applications. Journal of Materials Chemistry C, 2018, 6, 1959-1970.	2.7	8
22	Luminescent Dinuclear Copper(I) Complexes as Potential Thermally Activated Delayed Fluorescence (TADF) Emitters: A Theoretical Study. Journal of Physical Chemistry A, 2018, 122, 1413-1421.	1.1	34
23	Pairing-up viologen cations and dications: a microscopic investigation of van der Waals interactions. Physical Chemistry Chemical Physics, 2018, 20, 27878-27884.	1.3	10
24	Absorption Spectroscopy and Photophysics of a Re^Iâ€dppz Probe for DNAâ€Mediated Charge Transport. Chemistry - A European Journal, 2018, 24, 14425-14435.	1.7	9
25	Cooperativity in Spin Crossover Systems. An Atomistic Perspective on the Devilâ€™s Staircase. Inorganic Chemistry, 2018, 57, 9478-9488.	1.9	28
26	A Spin-Crossover Molecular Material Describing Four Distinct Thermal Pathways. Inorganic Chemistry, 2018, 57, 11019-11026.	1.9	19
27	Spin State Chemistry: Modulation of Ligand p<i>K</i>_a by Spin State Switching in a [2Ã—2] Iron(II) Grid-Type Complex. Journal of the American Chemical Society, 2018, 140, 8218-8227.	6.6	63
28	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
29	Electron transport through a spin crossover junction. Perspectives from a wavefunction-based approach. Journal of Chemical Physics, 2017, 146, 064112.	1.2	9
30	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
31	Twisting induces ferromagnetism in homometallic clusters. Dalton Transactions, 2017, 46, 11154-11158.	1.6	1
32	A probe of steric ligand substituent effects on the spin crossover of Fe(<scp>ii</scp>) complexes. Inorganic Chemistry Frontiers, 2017, 4, 1374-1383.	3.0	28
33	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
34	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
35	Understanding the Influence of the Electronic Structure on the Crystal Structure of a TTF-PTM Radical Dyad. Journal of Physical Chemistry A, 2016, 120, 10297-10303.	1.1	5
36	Three Redox States of a Diradical Acceptorâ€“Donorâ€“Acceptor Triad: Gating the Magnetic Coupling and the Electron Delocalization. Journal of Physical Chemistry Letters, 2016, 7, 2234-2239.	2.1	24

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37	Designed intramolecular blocking of the spin crossover of an Fe(<scp>ii</scp>) complex. Dalton Transactions, 2016, 45, 14058-14062.	1.6	15
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	The origin of the antiferromagnetic behaviour of the charge-transfer compound (HMTTF)[Ni(mnt)₂]. Dalton Transactions, 2015, 44, 608-614.	1.6	5
40	Dynamical effects on the magnetic properties of dithiazolyl bistable materials. Chemical Science, 2015, 6, 2371-2381.	3.7	34
41	Towards the tailored design of benzotriazinyl-based organic radicals displaying a spin transition. Chemical Communications, 2015, 51, 15776-15779.	2.2	16
42	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
43	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
44	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
45	The polymorphism of a triarylphosphine oxide: a case of missing isomers. CrystEngComm, 2014, 16, 8214-8223.	1.3	1
46	The key role of vibrational entropy in the phase transitions of dithiazolyl-based bistable magnetic materials. Nature Communications, 2014, 5, 4411.	5.8	55
47	Linear or Cyclic Clusters of Cu(II) with a Hierarchical Relationship. Inorganic Chemistry, 2014, 53, 3290-3297.	1.9	16
48	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
49	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
50	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
51	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
52	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
53	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
54	A molecular dynamics simulation of methane adsorption in single walled carbon nanotube bundles. Carbon, 2011, 49, 4544-4553.	5.4	46