Fernando Mota

List of Publications by Year in descending order

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42 papers	1,464 citations	304743 22 h-index	315739 38 g-index
43 all docs	43 docs citations	43 times ranked	1537 citing authors

#	Article	IF	Citations
1	Origin of the magnetic couplings for the weak ferromagnet Li+[TCNE]â€¢- (TCNEÂ=ÂTetracyanoethylene). Polyhedron, 2022, 221, 115871.	2.2	0
2	Reorganization of Intermolecular Interactions in the Polymorphic Phase Transition of a Prototypical Dithiazolyl-Based Bistable Material. Crystal Growth and Design, 2019, 19, 2329-2339.	3.0	7
3	A New Conformation With an Extraordinarily Long, 3.04â€…Ã… Twoâ€Electron, Sixâ€Center Bond Observed for the Ï€â€[TCNE]‹sub›2‹/sub›‹sup›2â¯‹/sup› Dimer in [NMe‹sub›4‹/sub›]‹sub›2‹/sub›[TCNE]‹sub›2‹/sub› (TCNE=Tetracyanoethylene). Chemistry - A European Journal, 2015, 21, 13240-13245.	3.3	9
4	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.	13.7	20
5	Diradicals acting through diamagnetic phenylene vinylene bridges: Raman spectroscopy as a probe to characterize spin delocalization. Journal of Chemical Physics, 2014, 140, 164903.	3.0	6
6	The key role of vibrational entropy in the phase transitions of dithiazolyl-based bistable magnetic materials. Nature Communications, 2014, 5, 4411.	12.8	55
7	Impact of short and long-range effects on the magnetic interactions in neutral organic radical-based materials. Physical Chemistry Chemical Physics, 2013, 15, 6982.	2.8	18
8	Evidence for Multicenter Bonding in Dianionic Tetracyanoethylene Dimers by Raman Spectroscopy. Angewandte Chemie - International Edition, 2013, 52, 6421-6425.	13.8	33
9	Evidence for Multicenter Bonding in Dianionic Tetracyanoethylene Dimers by Raman Spectroscopy. Angewandte Chemie, 2013, 125, 6549-6553.	2.0	13
10	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
11	Tunneling versus Hopping in Mixed-Valence Oligo-‹i›p‹/i›-phenylenevinylene Polychlorinated Bis(triphenylmethyl) Radical Anions. Journal of the American Chemical Society, 2011, 133, 5818-5833.	13.7	81
12	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
13	Comparative Analysis of the Multicenter, Long Bond in [TCNE]‹sup›Â·â¯‹/sup›and Phenalenyl Radical Dimers: A Unified Description of Multicenter, Long Bonds. Journal of the American Chemical Society, 2009, 131, 7699-7707.	13.7	122
14	The origin of the two-electron/four-centers Cï£¿C bond in Ï€-TCNE22â¯ dimers: Electrostatic or dispersion?. Journal of Computational Chemistry, 2007, 28, 326-334.	3.3	37
15	The Nature of the Câ€“HÂ·ÂÂ·ÂÂ·X Intermolecular Interactions in Molecular Crystals. A Theoretical Perspective. , 2006, , 193-244.		12
16	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.	1.7	20
17	Oâ¯Hâ‹…â‹…â‹…O Interactions Involving Doubly Charged Anions: Charge Compression in Carbonateâ€“Bicarbonate Crystals Queries on the theoretical part should be addressed to Professor J. J. Novoa.. Chemistry - A European Journal, 2002, 8, 1173.	3.3	35
18	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.	3.9	15

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19	Interanionic(â^')Oâ^'Hâ‹…â‹…â‹…O(â^') Interactions: A Solid-State and Computational Study of the Ring and Chain Motifs. Chemistry - A European Journal, 2000, 6, 4536-4551.	3.3	44
20	The Câ€“Hâ‹¯Ï€ bonds: strength, identification, and hydrogen-bonded nature: a theoretical study. Chemical Physics Letters, 2000, 318, 345-354.	2.6	157
21	Spin Density Distribution of Î±-Nitronyl Aminoxyl Radicals from Experimental and ab Initio Calculated ESR Isotropic Hyperfine Coupling Constants. Journal of the American Chemical Society, 2000, 122, 11393-11405.	13.7	70
22	Determination of the Spin Distribution in Nitronylnitroxides by Solid-State 1H, 2H, and 13C NMR Spectroscopy. Journal of the American Chemical Society, 1999, 121, 9659-9667.	13.7	66
23	Are non-linear Câ€“Hâ‹¯O contacts hydrogen bonds or Van der Waals interactions?. Chemical Physics Letters, 1998, 290, 519-525.	2.6	65
24	Câ€“HÂ·Â·Â·O Hydrogen bonds in the mixed-valence salt [(Î·6-C6H6)2Cr]+[CrO3(OCH3)]- and the breakdown of the length/strength analogy. New Journal of Chemistry, 1998, 22, 755-757.	2.8	37
25	Structure of the First Solvation Shell of the Hydroxide Anion. A Model Study Using OH-(H2O)n(n= 4, 5,) Tj ETQq1 1 0.784314 rgBT /Ov	2.5	79
26	Substituent effects in intermolecular C(sp3)-H â‹¯ O(sp3) contacts: how strong can a C(sp3)-H â‹¯ O(sp3) hydrogen bond be?. Chemical Physics Letters, 1997, 266, 23-30.	2.6	57
27	The symmetry breaking problem in the triflouride anion: A multireference approach. Journal of Chemical Physics, 1996, 105, 8777-8784.	3.0	25
28	Ab Initio Computation of the Spin Population of Substituted Î±-Nitronyl Nitroxide Radicals. Molecular Crystals and Liquid Crystals, 1995, 271, 79-90.	0.3	17
29	Pyramidality and metal-metal multiple bonding: structural correlations and theoretical study. Journal of the American Chemical Society, 1993, 115, 6216-6229.	13.7	44
30	Accurate calculation of the electron affinities of the group-13 atoms. Chemical Physics, 1992, 166, 77-84.	1.9	29
31	Interaction energies associated with short intermolecular contacts of carbon-hydrogen bonds. 1. Ab initio computational study of C-H.cntdot..cntdot..cntdot.anion interactions, C-H.cntdot..cntdot..cntdot.X-(X- = I3-, IBr2-, ICl2-). Inorganic Chemistry, 1991, 30, 54-58.	4.0	24
32	Mono- and multireference Moller-Plesset computation of the electron affinity. A full configuration interaction analysis on first-row atoms and their hydrides. The Journal of Physical Chemistry, 1991, 95, 3096-3105.	2.9	16
33	A full-CI analysis of the single- and multi-reference MÃ¸llerâ€"Plesset methods for the computation of electron affinities. Chemical Physics Letters, 1990, 165, 503-512.	2.6	10
34	The large range of chromium-chromium quadruple bond distances: structural and theoretical analysis. Journal of the American Chemical Society, 1990, 112, 8998-9000.	13.7	26
35	Structure and stability of the X3- systems (X = fluoride, chloride, bromide, iodide) and their interaction with cations. The Journal of Physical Chemistry, 1988, 92, 6561-6566.	2.9	54
36	Structure and stability of tetraatomic bromine and ion, Br4 and Br42-, and their interaction with cations and transition metals. Journal of the American Chemical Society, 1987, 109, 6586-6591.	13.7	17

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37	On the computation of molecular electronic affinities. Theoretica Chimica Acta, 1987, 72, 325-331.	0.8	5
38	Theoretical study of the vibrational-rotational spectra of diatomic molecules: A quantum chemistry experiment. Journal of Chemical Education, 1986, 63, 919.	2.3	4
39	Accurate electron affinities of several diatomic and triatomic molecules. Chemical Physics Letters, 1986, 123, 399-401.	2.6	15
40	The mechanism of electrical conductivity along polyhalide chains. Chemical Physics Letters, 1986, 132, 531-534.	2.6	12
41	Electron affinities: Basis and correlation effects. Chemical Physics Letters, 1985, 119, 135-140.	2.6	15
42	Theoretical Study of the Electronic Structure and Magnetic Interactions in Purely Organic Nitronyl Nitroxide Crystals. , 0, , 65-117.		1