

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	The C-H bonds: strength, identification, and hydrogen-bonded nature: a theoretical study. <i>Chemical Physics Letters</i> , 2000, 318, 345-354.	2.6	157
2	Comparative Analysis of the Multicenter, Long Bond in [TCNE] ^{•-} and Phenalenyl Radical Dimers: A Unified Description of Multicenter, Long Bonds. <i>Journal of the American Chemical Society</i> , 2009, 131, 7699-7707.	13.7	122
3	Tunneling versus Hopping in Mixed-Valence Oligo- <i>p</i> -phenylenevinylene Polychlorinated Bis(triphenylmethyl) Radical Anions. <i>Journal of the American Chemical Society</i> , 2011, 133, 5818-5833.	13.7	81
4	Structure of the First Solvation Shell of the Hydroxide Anion. A Model Study Using OH-(H ₂ O) _n (n= 4, 5). <i>J. Phys. Chem. B</i> , 2005, 109, 7979-7984.	2.5	79
5	Spin Density Distribution of \pm -Nitronyl Aminoxyl Radicals from Experimental and ab Initio Calculated ESR Isotropic Hyperfine Coupling Constants. <i>Journal of the American Chemical Society</i> , 2000, 122, 11393-11405.	13.7	70
6	Determination of the Spin Distribution in Nitronyl Nitroxides by Solid-State ¹ H, ² H, and ¹³ C NMR Spectroscopy. <i>Journal of the American Chemical Society</i> , 1999, 121, 9659-9667.	13.7	66
7	Are non-linear C-H...O contacts hydrogen bonds or Van der Waals interactions?. <i>Chemical Physics Letters</i> , 1998, 290, 519-525.	2.6	65
8	Origin of the Magnetic Bistability in Molecule-Based Magnets: A First-Principles Bottom-Up Study of the TTTA Crystal. <i>Journal of the American Chemical Society</i> , 2010, 132, 17817-17830.	13.7	61
9	Substituent effects in intermolecular C(sp ³)-H...O(sp ³) contacts: how strong can a C(sp ³)-H...O(sp ³) hydrogen bond be?. <i>Chemical Physics Letters</i> , 1997, 266, 23-30.	2.6	57
10	The key role of vibrational entropy in the phase transitions of dithiazolyl-based bistable magnetic materials. <i>Nature Communications</i> , 2014, 5, 4411.	12.8	55
11	Structure and stability of the X ⁻ systems (X = fluoride, chloride, bromide, iodide) and their interaction with cations. <i>The Journal of Physical Chemistry</i> , 1988, 92, 6561-6566.	2.9	54
12	Pyramidity and metal-metal multiple bonding: structural correlations and theoretical study. <i>Journal of the American Chemical Society</i> , 1993, 115, 6216-6229.	13.7	44
13	Interanionic(O ^{•-})...O...O(O ^{•-}) Interactions: A Solid-State and Computational Study of the Ring and Chain Motifs. <i>Chemistry - A European Journal</i> , 2000, 6, 4536-4551.	3.3	44
14	C-H...O Hydrogen bonds in the mixed-valence salt [(η -6-C ₆ H ₆) ₂ Cr] ⁺ [CrO ₃ (OCH ₃)] ⁻ and the breakdown of the length/strength analogy. <i>New Journal of Chemistry</i> , 1998, 22, 755-757.	2.8	37
15	The origin of the two-electron/four-centers C-C bond in TCNE dimers: Electrostatic or dispersion?. <i>Journal of Computational Chemistry</i> , 2007, 28, 326-334.	3.3	37
16	O...H...O Interactions Involving Doubly Charged Anions: Charge Compression in Carbonate/Bicarbonate Crystals. Queries on the theoretical part should be addressed to Professor J. J. Novoa. <i>Chemistry - A European Journal</i> , 2002, 8, 1173.	3.3	35
17	Evidence for Multicenter Bonding in Dianionic Tetracyanoethylene Dimers by Raman Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 6421-6425.	13.8	33
18	Accurate calculation of the electron affinities of the group-13 atoms. <i>Chemical Physics</i> , 1992, 166, 77-84.	1.9	29

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19	Synthesis, Structure, Magnetic Behavior, and Theoretical Analysis of Diazine-Bridged Magnetic Ladders: Cu(quinoline) ₂ and Cu(2,3-dimethylpyrazine) ₂ (X = Cl, Br). <i>Inorganic Chemistry</i> , 2012, 51, 6315-6325.	4.0	27
20	The large range of chromium-chromium quadruple bond distances: structural and theoretical analysis. <i>Journal of the American Chemical Society</i> , 1990, 112, 8998-9000.	13.7	26
21	The symmetry breaking problem in the trifluoride anion: A multireference approach. <i>Journal of Chemical Physics</i> , 1996, 105, 8777-8784.	3.0	25
22	Interaction energies associated with short intermolecular contacts of carbon-hydrogen bonds. 1. Ab initio computational study of C-H...anion interactions, C-H...X (X = I ⁻ , Br ⁻ , Cl ⁻). <i>Inorganic Chemistry</i> , 1991, 30, 54-58.	4.0	24
23	Bulk ferromagnetism in nitronyl nitroxide crystals: a first principles bottom-up comparative study of four bulk nitronyl nitroxide ferromagnets (KAXHAS, YOMYII, LICMIT and YUIJNEW). <i>Molecular Physics</i> , 2006, 104, 857-873.	1.7	20
24	Unravelling the Key Driving Forces of the Spin Transition in $\dot{\text{C}}\text{r}^{\text{II}}$ -Dimers of Spiro-biphenalenyl-Based Radicals. <i>Journal of the American Chemical Society</i> , 2015, 137, 12843-12855.	13.7	20
25	Impact of short and long-range effects on the magnetic interactions in neutral organic radical-based materials. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 6982.	2.8	18
26	Structure and stability of tetraatomic bromine and ion, Br ₄ and Br ₄ ²⁻ , and their interaction with cations and transition metals. <i>Journal of the American Chemical Society</i> , 1987, 109, 6586-6591.	13.7	17
27	Ab Initio Computation of the Spin Population of Substituted $\dot{\text{C}}\text{r}^{\text{II}}$ -Nitronyl Nitroxide Radicals. <i>Molecular Crystals and Liquid Crystals</i> , 1995, 271, 79-90.	0.3	17
28	Mono- and multireference Moller-Plesset computation of the electron affinity. A full configuration interaction analysis on first-row atoms and their hydrides. <i>The Journal of Physical Chemistry</i> , 1991, 95, 3096-3105.	2.9	16
29	Electron affinities: Basis and correlation effects. <i>Chemical Physics Letters</i> , 1985, 119, 135-140.	2.6	15
30	Accurate electron affinities of several diatomic and triatomic molecules. <i>Chemical Physics Letters</i> , 1986, 123, 399-401.	2.6	15
31	A general study of the spin population of $\dot{\text{C}}\text{r}^{\text{II}}$ -nitronyl nitroxide radicals: radicals with crystals presenting dominant ferro or antiferromagnetic behavior. <i>Synthetic Metals</i> , 2001, 122, 477-483.	3.9	15
32	Evidence for Multicenter Bonding in Dianionic Tetracyanoethylene Dimers by Raman Spectroscopy. <i>Angewandte Chemie</i> , 2013, 125, 6549-6553.	2.0	13
33	The mechanism of electrical conductivity along polyhalide chains. <i>Chemical Physics Letters</i> , 1986, 132, 531-534.	2.6	12
34	The Nature of the C-H...X Intermolecular Interactions in Molecular Crystals. A Theoretical Perspective. , 2006, , 193-244.		12
35	A full-CI analysis of the single- and multi-reference Moller-Plesset methods for the computation of electron affinities. <i>Chemical Physics Letters</i> , 1990, 165, 503-512.	2.6	10
36	A New Conformation With an Extraordinarily Long, 3.04 Å... Two-Electron, Six-Center Bond Observed for the $\dot{\text{C}}\text{r}^{\text{II}}$ [TCNE] ₂ ²⁺ Dimer in [NMe ₄] ₂ [TCNE] ₂ (TCNE=Tetracyanoethylene). <i>Chemistry - A European Journal</i> , 2015, 21, 13240-13245.	3.3	9

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37	Reorganization of Intermolecular Interactions in the Polymorphic Phase Transition of a Prototypical Dithiazolyl-Based Bistable Material. <i>Crystal Growth and Design</i> , 2019, 19, 2329-2339.	3.0	7
38	Diradicals acting through diamagnetic phenylene vinylene bridges: Raman spectroscopy as a probe to characterize spin delocalization. <i>Journal of Chemical Physics</i> , 2014, 140, 164903.	3.0	6
39	On the computation of molecular electronic affinities. <i>Theoretica Chimica Acta</i> , 1987, 72, 325-331.	0.8	5
40	Theoretical study of the vibrational-rotational spectra of diatomic molecules: A quantum chemistry experiment. <i>Journal of Chemical Education</i> , 1986, 63, 919.	2.3	4
41	Theoretical Study of the Electronic Structure and Magnetic Interactions in Purely Organic Nitronyl Nitroxide Crystals. , 0, , 65-117.		1
42	Origin of the magnetic couplings for the weak ferromagnet Li+[TCNE]â€¢- (TCNE=â€¢Tetracyanoethylene). <i>Polyhedron</i> , 2022, 221, 115871.	2.2	0