Fanica Cimpoesu

List of Publications by Year
in descending order

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69 papers	1,476 citations	304368 22 h-index	329751 37 g-index
70 all docs	70 docs citations	70 times ranked	1673 citing authors

#	Article	IF	Citations
1	Characterizing the EâŠ—e Jahnâ€“Teller Potential Energy Surfaces by Differential Geometry Tools. Symmetry, 2022, 14, 436.	1.1	1
2	The Density Functional Theory Account of Interplaying Long-Range Exchange and Dispersion Effects in Supramolecular Assemblies of Aromatic Hydrocarbons with Spin. Molecules, 2022, 27, 45.	1.7	1
3	New Syntheses, Analytic Spin Hamiltonians, Structural and Computational Characterization for a Series of Tri-, Hexa- and Hepta-Nuclear Copper (II) Complexes with Prototypic Patterns. Chemistry, 2021, 3, 411-439.	0.9	3
4	The angular overlap model of ligand field theory for f elements: An intuitive approach building bridges between theory and experiment. Coordination Chemistry Reviews, 2021, 441, 213981.	9.5	17
5	Intra- and Inter-Molecular Spin Coupling in Phenalenyl Dimeric Systems. Journal of Physical Chemistry A, 2021, 125, 6893-6901.	1.1	7
6	Molecular and Supramolecular Interactions in Systems with Nitroxide-Based Radicals. International Journal of Molecular Sciences, 2019, 20, 4733.	1.8	6
7	Valence Bond Account of Triangular Polyaromatic Hydrocarbons with Spin: Combining Ab Initio and Phenomenological Approaches. Journal of Physical Chemistry C, 2019, 123, 6869-6880.	1.5	18
8	Atoms in Generalized Orbital Configurations: Towards Atom-Dedicated Density Functionals. International Journal of Molecular Sciences, 2019, 20, 5943.	1.8	4
9	Spin Coupling and Magnetic Anisotropy in 1D Complexes with Manganese(III) Units and Carboxylate Bridges â€“ Synthesis, Analysis, Calculations, and Models. European Journal of Inorganic Chemistry, 2018, 2018, 1409-1418.	1.0	1
10	New Keys for Old Keywords: Hybridization and Aromaticity, Graphs and Topology. , 2018, , 389-501.		0
11	Coordination Bonding: Electronic Structure and Properties. , 2018, , 503-612.		1
12	The Modeling in Molecular Magnetism. , 2018, , 613-679.		0
13	Bonding in Rings and Clusters. , 2018, , 681-723.		0
14	Wave Function Theories and Electronic Structure Methods: Quantum Chemistry, from Atoms to Molecules. , 2018, , 107-220.		0
15	Electron Transfer and Dye Regeneration in Dye-Sensitized Solar Cells. , 2018, , .		0
16	Properties Design: Prediction and Experimental Validation of the Luminescence Properties of a New Eu^{II}â€Based Phosphor. Chemistry - A European Journal, 2018, 24, 16276-16281.	1.7	11
17	Electronic Structure of Linear Polyacenes. Current Organic Chemistry, 2018, 21, .	0.9	1
18	Ferroelectric polarization of hydroxyapatite from density functional theory. RSC Advances, 2017, 7, 21375-21379.	1.7	37

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19	On The Density Functional Theory Treatment of Lanthanide Coordination Compounds: A Comparative Study in a Series of Cuâ€“Ln (Ln = Gd, Tb, Lu) Binuclear Complexes. Inorganic Chemistry, 2017, 56, 9474-9485.	1.9	22
20	The Spin Coupling in the Polyaromatic Hydrocarbons and Carbon-Based Materials. , 2017, , 327-371.		5
21	Case Studies in the Challenge of Properties Design at Nanoscale. Advances in Chemical and Materials Engineering Book Series, 2017, , 148-184.	0.2	0
22	Noble gas endohedral fullerenes, Ng@C60 (Ng=Ar, Kr): a particular benchmark for assessing the account of non-covalent interactions by density functional theory calculations. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	11
23	Lone-Pair-Electron-Driven Ionic Displacements in a Ferroelectric Metalâ€“Organic Hybrid. Inorganic Chemistry, 2016, 55, 10337-10342.	1.9	51
24	Monte Carlo Simulations of the Magnetic Behavior, Ordering Temperature and Magnetocaloric Effects in 1D, 2D and 3D Ferrimagnetic Systems. Journal of Nanoscience and Nanotechnology, 2015, 15, 263-268.	0.9	2
25	On exchange coupling and bonding in the Gd₂@C₈₀ and Gd₂@C₇₉N endohedral dimetallo-fullerenes. Molecular Physics, 2015, 113, 1712-1727.	0.8	17
26	A ligand field theory-based methodology for the characterization of the Eu 2+ [Xe]4f 6 5d 1 excited states in solid state compounds. Chemical Physics Letters, 2015, 622, 120-123.	1.2	14
27	Tailoring the optical properties of lanthanide phosphors: prediction and characterization of the luminescence of Pr³⁺-doped LiYF₄. Physical Chemistry Chemical Physics, 2015, 17, 9116-9125.	1.3	18
28	Development and applications of the LFDFT: the non-empirical account of ligand field and the simulation of the fâ€“d transitions by density functional theory. Physical Chemistry Chemical Physics, 2015, 17, 18547-18557.	1.3	23
29	Prospecting Lighting Applications with Ligand Field Tools and Density Functional Theory: A First-Principles Account of the 4f⁷â€“4f⁶5d¹ Luminescence of CsMgBr₃:Eu²⁺. Inorganic Chemistry, 2015, 54, 8319-8326.	1.9	39
30	Metal-Organic Frameworks with dâ€“f Cyanide Bridges: Structural Diversity, Bonding Regime, and Magnetism. Structure and Bonding, 2014, , 185-229.	1.0	11
31	The theoretical account of the ligand field bonding regime and magnetic anisotropy in the DySc₂N@C₈₀ single ion magnet endohedral fullerene. Physical Chemistry Chemical Physics, 2014, 16, 11337-11348.	1.3	36
32	Ligand field density functional theory for the prediction of future domestic lighting. Physical Chemistry Chemical Physics, 2014, 16, 14625-14634.	1.3	24
33	Ab initio study of exchange coupling for the consistent understanding of the magnetic ordering at room temperature in V[TCNE] x. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	9
34	The angular overlap model extended for two-open-shell f and d electrons. Physical Chemistry Chemical Physics, 2014, 16, 12282-12290.	1.3	28
35	Disorder, exchange and magnetic anisotropy in the room-temperature molecular magnet V[TCNE]x â€“ A theoretical study. Computational Materials Science, 2014, 91, 320-328.	1.4	11
36	New insights in the bonding regime and ligand field in Wernerian complexes. A density functional study. Polyhedron, 2013, 52, 183-195.	1.0	5

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37	Ligand field density functional theory calculation of the 4f2 â†' 4f15d1 transitions in the quantum cutter Cs2KYF6:Pr3+. Physical Chemistry Chemical Physics, 2013, 15, 13902.	1.3	50
38	Calculation of the 4f1â†'4f05d1 transitions in Ce3+-doped systems by Ligand Field Density Functional Theory. Chemical Physics Letters, 2013, 588, 260-266.	1.2	36
39	Comparative computational IR, Raman and phosphorescence study of Ru- and Rh-based complexes. Molecular Physics, 2013, 111, 1526-1538.	0.8	6
40	Density Functional Theory (DFT) Study of Coumarin-based Dyes Adsorbed on TiO2 Nanoclustersâ€"Applications to Dye-Sensitized Solar Cells. Materials, 2013, 6, 2372-2392.	1.3	74
41	DFT Study of Binding and Electron Transfer from a Metal-Free Dye with Carboxyl, Hydroxyl, and Sulfonic Anchors to a Titanium Dioxide Nanocluster. International Journal of Photoenergy, 2013, 2013, 1-15.	1.4	23
42	Structure and Magnetism in Feâ€"Gd Based Dinuclear and Chain Systems. The Interplay of Weak Exchange Coupling and Zero Field Splitting Effects. Inorganic Chemistry, 2012, 51, 40-50.	1.9	27
43	Chiral Crystallization of a Heterodinuclear Ni-Ln Series: Comprehensive Analysis of the Magnetic Properties.. Inorganic Chemistry, 2012, 51, 11279-11293.	1.9	72
44	Broken symmetry DFT calculations of exchange coupling constants for manganeseâ€"porphyrin quasi-one-dimensional molecular magnets. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	8
45	Vibrational properties of noble gas endohedral fullerenes. Physical Chemistry Chemical Physics, 2011, 13, 9609.	1.3	22
46	Rationalization of the Lanthanide-Ion-Driven Magnetic Properties in a Series of 4fâ€"5d Cyano-Bridged Chains. Inorganic Chemistry, 2011, 50, 9678-9687.	1.9	23
47	DFT study of structureâ€"properties correlations in [MnTPP][TCNE] quasi-one-dimensional molecular magnets. Theoretical Chemistry Accounts, 2011, 129, 847-857.	0.5	8
48	Influence of surface chemistry on the electronic properties of graphene nanoflakes. Chemical Physics Letters, 2011, 503, 91-96.	1.2	24
49	Theoretical Calculations of Structure and Exchange Coupling of a Room-Temperature Molecular Magnet. , 2010, , .		0
50	Noncovalent effects in the coordination and assembling of the[Fe(bpca)2][Er(NO3)3(H2O)4]NO3 system. Open Chemistry, 2010, 8, 519-529.	1.0	7
51	Magnetic anisotropy and molecular assembling in d complex cationâ€"f complex anion type coordination compounds. Solid State Sciences, 2009, 11, 760-765.	1.5	9
52	The association of dehydro-epiandrosterone and adenosine triphosphate acid: A DFT study of interactions between prototypic biologically active molecules. Computational and Theoretical Chemistry, 2009, 912, 32-37.	1.5	2
53	The DFT rationalization of exchange and anisotropy in one-dimensional d-p magnets: The [MnIII(porphyrin)][TCNE] case study. Polyhedron, 2009, 28, 2039-2043.	1.0	10
54	Monte Carlo simulation of magnetic ordering in the Gd3Fe5O12 Ising ferrite with garnet structure. Journal of Magnetism and Magnetic Materials, 2008, 320, 2149-2154.	1.0	6

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55	Geometry, bonding and magnetism in planar triangulene graphene molecules with D3h symmetry: Zigzag (m=2,â€¦15), Chemical Physics, 2008, 354, 1-15.	0.9	47
56	Bonding and Magnetism in High Symmetry Nano-Sized Graphene Molecules: Linear Acenes C_{4<I>m</I>+2}H_{2<I>m</I>+4} (<I>m</I>=2,…25); Zigzag Hexangulenes C_{6<I>m</I>^{**}2}H_{6<I>m</I>} (<I>m</I>=2,…10); Crenelated Hexangulenes C_{6(3<I>m</I>^{**}2−3<I>m</I>+1)}H_{6(2<I>m</I>−1)} (<I>m</I>=2,…6); Zigzag Triangulenes C_{<I>m</I>^{**}2+4<I>m</I>+1}H<SUB>	0.4	23
57	Spin Coupling in the Supramolecular Structure of a New Tetra(Quinolineâ¯TEMPO)Yttrium(III) Complex. Inorganic Chemistry, 2007, 46, 660-669.	1.9	6
58	Computational study of the molecular complexes between cholesterol and two isomers of the pralidoxime (PAM). Computational and Theoretical Chemistry, 2007, 813, 3-8.	1.5	0
59	The magnetic anisotropy and assembling of the lanthanide coordination units in [Fe(bpca)2][Er(NO3)3(H2O)4]NO3. Polyhedron, 2007, 26, 2069-2073.	1.0	10
60	AÂBinuclearÂFe(III)Dy(III)ÂSingleÂMoleculeÂMagnet.ÂQuantumÂEffectsÂandÂModels. Journal of the American Chemical Society, 2006, 128, 9008-9009.	6.6	252
61	Theoretical study of DHEA: comparative HF and DFT calculations of the electronic properties of a complex between DHEA and serotonin. Journal of Molecular Modeling, 2006, 12, 146-151.	0.8	8
62	A MONTE CARLO SIMULATION OF MAGNETIC ORDERING IN ISING FERRITES OF FORMULA 5Fe2O3.3Y2O3 WITH GARNET STRUCTURE. Journal of Theoretical and Computational Chemistry, 2006, 05, 151-161.	1.8	3
63	New Keys for Old Keywords. Case Studies within the Updated Paradigms of the Hybridization and Aromaticity. Monatshefte FÃ¼r Chemie, 2005, 136, 1071-1085.	0.9	3
64	Mechanism of Ferromagnetic Coupling in Copper(II)-Gadolinium(III) Complexes. Journal of the American Chemical Society, 2004, 126, 3321-3331.	6.6	141
65	Synthesis, Structural Characterization, and Theoretical Treatment of an Unusual Organozirconium Hydroxide with the [Zr6(Î¼4-O)(Î¼-O)4(Î¼-OH)8] Coreâ€. Organometallics, 2003, 22, 3034-3038.	1.1	23
66	Lightest Member of the Basic Carboxylate Structural Pattern:Â [Al3(Î¼3-O)(Î¼-O2CCF3)6(THF)3][(Me3Si)3CAl(O2CCF3)3]Â·C7H8. Inorganic Chemistry, 2002, 41, 1022-1025.	1.9	24
67	Syntheses, Structures, and Surface Aromaticity of the New Carbaalane [(AlH)6(AlNMe3)2(CCH2R)6] (R =) Tj ETQq1 1 0.784314 rgBT O of the American Chemical Society, 2002, 124, 5441-5448.	6.6	59
68	New Synthetic and Structural Aspects in the Chemistry of Alkylaluminum Fluorides. The Mutual Influence of Hard and Soft Ligands and the Hybridization as Rigorous Structural Criterion#. Inorganic Chemistry, 2001, 40, 4947-4955.	1.9	28
69	On the thermal stability and non-isothermal decomposition kinetics of some coordination compounds of cobalt, nickel and copper with a Î²-dicarbonylic compound and 4-benzoylpyridine or 4,4'-dipyridyl as ligands. Thermochimica Acta, 1993, 221, 237-253.	1.2	2