Pere Alemany

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3898838/publications.pdf

Version: 2024-02-01

184	11,132	47006	30087
papers	citations	47	103
		h-index	g-index

198	198	198	8748
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Shape maps and polyhedral interconversion paths in transition metal chemistry. Coordination Chemistry Reviews, 2005, 249, 1693-1708.	18.8	889
2	Broken symmetry approach to calculation of exchange coupling constants for homobinuclear and heterobinuclear transition metal complexes. Journal of Computational Chemistry, 1999, 20, 1391-1400.	3.3	836
3	Toward the Prediction of Magnetic Coupling in Molecular Systems:â€‰ Hydroxo- and Alkoxo-Bridged Cu(II) Binuclear Complexes. Journal of the American Chemical Society, 1997, 119, 1297-1303.	13.7	816
4	The Rich Stereochemistry of Eight-Vertex Polyhedra: A Continuous Shape Measures Study. Chemistry - A European Journal, 2005, 11, 1479-1494.	3.3	729
5	Magnetic Coupling in End-On Azido-Bridged Transition Metal Complexes:Â A Density Functional Study. Journal of the American Chemical Society, 1998, 120, 11122-11129.	13.7	676
6	About the calculation of exchange coupling constants in polynuclear transition metal complexes. Journal of Computational Chemistry, 2003, 24, 982-989.	3.3	472
7	Structural Modeling and Magnetoâ^'Structural Correlations for Hydroxo-Bridged Copper(II) Binuclear Complexes. Inorganic Chemistry, 1997, 36, 3683-3688.	4.0	386
8	Minimal Distortion Pathways in Polyhedral Rearrangements. Journal of the American Chemical Society, 2004, 126, 1755-1763.	13.7	362
9	Distortions in Octahedrally Coordinated d0Transition Metal Oxides:Â A Continuous Symmetry Measures Approach. Chemistry of Materials, 2006, 18, 3176-3183.	6.7	326
10	Exchange Coupling in Carboxylato-Bridged Dinuclear Copper(II) Compounds: A Density Functional Study. Chemistry - A European Journal, 2001, 7, 627-637.	3.3	325
11	Shape and Symmetry of Heptacoordinate Transition-Metal Complexes: Structural Trends. Chemistry - A European Journal, 2003, 9, 1281-1295.	3.3	225
12	Exchange Coupling in Oxalato-Bridged Copper(II) Binuclear Compounds: A Density Functional Study. Chemistry - A European Journal, 1998, 4, 476-484.	3.3	197
13	Local Aromaticity of [n]Acenes, [n]Phenacenes, and [n]Helicenes (n = 1â^'9). Journal of Organic Chemistry, 2005, 70, 2509-2521.	3.2	195
14	Mapping the Stereochemistry and Symmetry of Tetracoordinate Transition-Metal Complexes. Chemistry - A European Journal, 2004, 10, 190-207.	3.3	175
15	Electronic structure and properties of AlN. Physical Review B, 1994, 49, 7115-7123.	3.2	146
16	Electronic structure and properties ofCu2O. Physical Review B, 1997, 56, 7189-7196.	3.2	146
17	Calculation of exchange coupling constants in solid state transition metal compounds using localized atomic orbital basis sets. Journal of Solid State Chemistry, 2003, 176, 400-411.	2.9	135
18	To Bend or Not To Bend:Â Dilemma of the Edge-Sharing Binuclear Square Planar Complexes of d8Transition Metal Ions. Inorganic Chemistry, 1998, 37, 804-813.	4.0	126

#	Article	IF	Citations
19	Exchange Coupling in Halo-Bridged Dinuclear Cu(II) Compounds:Â A Density Functional Study. Inorganic Chemistry, 2002, 41, 3769-3778.	4.0	118
20	Density functional study of magnetostructural correlations in cubane complexes containing the Cu4O4core. Journal of Materials Chemistry, 2006, 16, 2729-2735.	6.7	107
21	On the Bonding Nature of the M.cntdot. .cntdot. .cntdot.M Interactions in Dimers of Square-Planar Pt(II) and Rh(I) Complexes. Journal of the American Chemical Society, 1995, 117, 7169-7171.	13.7	103
22	Continuous chirality measures in transition metal chemistry. Chemical Society Reviews, 2005, 34, 313.	38.1	98
23	Electronic Structure and Bonding in CuMO2 (M = Al, Ga, Y) Delafossite-Type Oxides:â€‰ An Ab Initio Study. Journal of Physical Chemistry B, 1999, 103, 8060-8066.	2.6	95
24	Density functional study of the exchange coupling in distorted cubane complexes containing the Cu4O4 core. Polyhedron, 2001, 20, 1323-1327.	2.2	90
25	Analytical methods for calculating Continuous Symmetry Measures and the Chirality Measure. Journal of Computational Chemistry, 2008, 29, 2712-2721.	3.3	89
26	â€œAggregation-induced emissionâ€•of transition metal compounds: Design, mechanistic insights, and applications. Journal of Photochemistry and Photobiology C: Photochemistry Reviews, 2019, 41, 100317.	11.6	85
27	Density Functional Calculations of NMR Chemical Shifts with the Inclusion of Spinâ^'Orbit Coupling in Tungsten and Lead Compounds. Journal of Physical Chemistry A, 1999, 103, 8288-8294.	2.5	82
28	Essential role of anions in the charge ordering transition of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-(BEDT-TTF)<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>I<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:	3.2	77
29	Color and Conductivity in Cu2O and CuAlO2:â€‰ A Theoretical Analysis of d10Â·Â·Â·d10 Interactions in Solid-State Compounds. Chemistry of Materials, 2001, 13, 338-344.	6.7	76
30	Electronic structure and bonding in skutterudite-type phosphides. Physical Review B, 1996, 53, 10605-10609.	3.2	74
31	Exchange Coupling in Cyano-Bridged Homodinuclear Cu(II) and Ni(II) Complexes:Â Synthesis, Structure, Magnetism, and Density Functional Theoretical Study. Inorganic Chemistry, 2001, 40, 5868-5877.	4.0	74
32	Electronic Structure and Magnetic Properties of CuFeS₂. Inorganic Chemistry, 2015, 54, 4840-4849.	4.0	69
33	Local Aromaticity of the Lowest-Lying Singlet States of [n]Acenes (n = 6â^'9). Journal of Physical Chemistry A, 2005, 109, 10629-10632.	2.5	68
34	Nature of Holes, Oxidation States, and Hypervalency in Covellite (CuS). Inorganic Chemistry, 2014, 53, 12402-12406.	4.0	68
35	Theoretical search for new ferromagnetically coupled transition metal complexes. Chemical Communications, 1998, , 2767-2768.	4.1	62
36	Theoretical study of the exchange coupling in copper(II) binuclear compounds with oxamidate and related polyatomic bridging ligandsâ€Šâ€. Journal of the Chemical Society Dalton Transactions, 1999, , 1669-1676.	1.1	61

#	Article	IF	Citations
37	Conducting Anilate-Based Mixed-Valence Fe(II)Fe(III) Coordination Polymer: Small-Polaron Hopping Model for Oxalate-Type Fe(II)Fe(III) 2D Networks. Journal of the American Chemical Society, 2018, 140, 12611-12621.	13.7	58
38	Role of Electron Density and Magnetic Couplings on the Nucleus-Independent Chemical Shift (NICS) Profiles of [2.2]Paracyclophane and Related Species. Journal of Organic Chemistry, 2006, 71, 1700-1702.	3.2	57
39	Metal-ceramic adhesion: quantum mechanical modeling of transition metal-alumina interfaces. The Journal of Physical Chemistry, 1993, 97, 8464-8475.	2.9	56
40	Electronic Structure and Magnetic Behavior in Polynuclear Transition-Metal Compounds. , 0, , 227-279.		55
41	Symmetry operation measures. Journal of Computational Chemistry, 2008, 29, 190-197.	3.3	55
42	New â€˜aggregation induced emission (AIE)â€™ active cyclometalated iridium(iii) based phosphorescent sensors: high sensitivity for mercury(ii) ions. Dalton Transactions, 2014, 43, 16431-16440.	3.3	54
43	Bonding and structure in L4M2(.mu.-XRn)2 diamonds of tetrahedral d10 ions. Effect of substituents on the M- -M interaction. Inorganic Chemistry, 1992, 31, 4266-4275.	4.0	52
44	Through-ring bonding in edge-sharing dimers of square planar complexes. Journal of Organometallic Chemistry, 1994, 478, 75-82.	1.8	52
45	On the Existence of a Pyramidality Effect in d8Â·Â·Â·d8Contacts. Theoretical Study and Structural Correlation. Inorganic Chemistry, 1996, 35, 5061-5067.	4.0	50
46	Facile tuning of the aggregation-induced emission wavelength in a common framework of a cyclometalated iridium(<scp>iii</scp>) complex: micellar encapsulated probe in cellular imaging. Journal of Materials Chemistry C, 2014, 2, 5615-5628.	5.5	49
47	Further Theoretical Evidence for the Exceptionally Strong Ferromagnetic Coupling in Oxo-Bridged Cu(II) Dinuclear Complexes. Journal of Physical Chemistry A, 2002, 106, 4938-4941.	2.5	48
48	Donorâ€“anion interactions in quarter-filled low-dimensional organic conductors. Materials Horizons, 2018, 5, 590-640.	12.2	47
49	Room-Temperature Synthesis and Crystal, Magnetic, and Electronic Structure of the First Silver Copper Oxide. Inorganic Chemistry, 2002, 41, 6604-6613.	4.0	44
50	Molecules and crystals with both icosahedral and cubic symmetry. Chemical Communications, 2008, , 2717.	4.1	43
51	Localization versus Delocalization in Chiral Single Component Conductors of Gold Bis(dithiolene) Complexes. Journal of the American Chemical Society, 2016, 138, 6838-6851.	13.7	43
52	Crystal Structure of the Host Lattices of the Superconductors LixMNX (M = Zr, Hf; X = Cl, Br). Chemistry of Materials, 1999, 11, 203-206.	6.7	42
53	Asymmetry and Magnetism in Bis(oximato)-Bridged Heterobimetallic Compounds: A Computational Approach. Chemistry - A European Journal, 2000, 6, 327-333.	3.3	41
54	Adhesion of rhodium, palladium, and platinum to alumina and the reduction of nitric oxide on the resulting surfaces: a theoretical analysis. The Journal of Physical Chemistry, 1993, 97, 7691-7699.	2.9	36

#	Article	IF	Citations
55	A Theoretical Study of the Exchange Coupling in Hydroxo- and Alkoxo-Bridged Dinuclear Oxovanadium(IV) Compounds. European Journal of Inorganic Chemistry, 2004, 2004, 143-153.	2.0	36
56	The electronic structure of barium gallium antimonide (Ba7Ga4Sb9): a compound seemingly probing the limits of the Zintl concept. Inorganic Chemistry, 1990, 29, 3070-3073.	4.0	33
57	Are nucleus-independent (NICS) and 1H NMR chemical shifts good indicators of aromaticity in Ï€-stacked polyfluorenes?. Chemical Physics Letters, 2006, 428, 191-195.	2.6	33
58	Electronic Structure and Bonding in CaC2. The Journal of Physical Chemistry, 1995, 99, 3114-3119.	2.9	32
59	Through-Ring Bonding in Edge Sharing Dimers of Octahedral Complexes. Inorganic Chemistry, 2000, 39, 3166-3175.	4.0	31
60	â€˜Aggregation induced emissionâ€™ active iridium(iii) complexes with applications in mitochondrial staining. RSC Advances, 2017, 7, 5642-5648.	3.6	31
61	Dual emission and multi-stimuli-response in iridium(<scp>iii</scp>) complexes with aggregation-induced enhanced emission: applications for quantitative CO₂ detection. Journal of Materials Chemistry C, 2017, 5, 7784-7798.	5.5	31
62	Toroidal nickel thiolates: structure and bonding. Journal of the American Chemical Society, 1993, 115, 8290-8297.	13.7	30
63	Origin of the Metal-to-Insulator Transition in H0.33MoO3. Inorganic Chemistry, 1997, 36, 4627-4632.	4.0	29
64	Roles of cations, electronegativity difference, and anionic interlayer interactions in the metallic versus nonmetallic character of Zintl phases related to arsenic. Journal of Computational Chemistry, 2008, 29, 2144-2153.	3.3	29
65	Association of two-coordinate copper(I) complexes: switching on and off CuÂ·Â·Â·Cu, ligandÂ·Â·Â·ligand and Cuâ€“ligand interactions. Chemical Communications, 1998, , 1149-1150.	4.1	28
66	Electronic structure and anion ordering in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mo>(</mml:mo><mml:mi) Tj ETQq0 0 0 rgBT /O xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>ClO</mml:mtext><mml:mn>4</mml:mn></mml:msub		

#	Article	IF	Citations
73	Microwave-assisted facile and expeditive syntheses of phosphorescent cyclometallated iridium(III) complexes. Polyhedron, 2013, 53, 286-294.	2.2	22
74	Evaluation of novel platinum(<scp>ii</scp>) based AIE compound-encapsulated mesoporous silica nanoparticles for cancer theranostic application. Dalton Transactions, 2018, 47, 4613-4624.	3.3	22
75	Concerning the Different Roles of Cations in Metallic Zintl Phases:â€‰ Ba7Ga4Sb9 as a Test Case. Inorganic Chemistry, 2006, 45, 7235-7241.	4.0	21
76	Charge ordering in low dimensional organic conductors: Structural aspects. Physica Status Solidi (B): Basic Research, 2012, 249, 937-942.	1.5	21
77	Polyhedral Interconversion Coupled with Proton Transfer between an Ammonium Cation and the [Co(CO)4]â^' Ion. Angewandte Chemie - International Edition, 2006, 45, 1457-1460.	13.8	19
78	Symmetry measures of the electron density. Journal of Computational Chemistry, 2010, 31, 2389-2404.	3.3	19
79	In Search of Chiral Molecular Superconductors: Îºâ€[(S,S)â€DMâ€BEDTâ€TTF]₂ClO₄ Revisited. Advanced Materials, 2020, 32, e2002811.	21.0	19
80	Electronic Structure, Chemical Bonding, and Jahn-Teller Distortions in CdPS3. Inorganic Chemistry, 1995, 34, 1159-1163.	4.0	18
81	Exchange coupling in Âµ-aqua:Âµ-oxo vs. di-Âµ-hydroxo dinuclear Cu(ii) compounds: a density functional study. Dalton Transactions, 2005, , 2624.	3.3	18
82	Links between the Crystal and Electronic Structure in the New Family of Unconventional Superconductors A2Cr3As3 (A = K, Rb, Cs). Inorganic Chemistry, 2015, 54, 8029-8034.	4.0	18
83	Rich Polymorphism of Layered NbS₃. Chemistry of Materials, 2021, 33, 5449-5463.	6.7	18
84	Stereochemistry of Complexes with Double and Triple Metalâ€“Ligand Bonds: A Continuous Shape Measures Analysis. Inorganic Chemistry, 2014, 53, 12151-12163.	4.0	17
85	Electronic Structure and Bonding in Tricoordinate Amido Complexes of Transition Metals. Inorganic Chemistry, 1999, 38, 707-715.	4.0	16
86	Theoretical approach to the magnetostructural correlations in the spin-Peierls compoundCuGeO3. Physical Review B, 2000, 61, 54-57.	3.2	16
87	Distortions of Ï€â€Coordinated Arenes with Anionic Character. Chemistry - A European Journal, 2014, 20, 14674-14689.	3.3	16
88	Self-Assembly of Discrete Metallocycles versus Coordination Polymers Based on Cu(I) and Ag(I) Ions and Flexible Ligands: Structural Diversification and Luminescent Properties. Polymers, 2016, 8, 46.	4.5	16
89	Structural and electronic control of the metal to insulator transition and local orderings in theÎ,-(BEDT-TTF)₂X organic conductors. Journal of Physics Condensed Matter, 2015, 27, 465702.	1.8	15
90	Electronic Structure and Dynamic Properties of Solid Alkali Cyanides. Journal of Physical Chemistry A, 1997, 101, 1393-1399.	2.5	14

#	Article	IF	Citations
91	Oxidation States, Transport Properties, and TeÂ·Â·Â·Te Short Contacts in the Ternary Transition Metal Tellurides Ta3Pd3Te14and Ta4Pd3Te16. Inorganic Chemistry, 1997, 36, 5050-5057.	4.0	14
92	Ligand effects and dimer formation in dicoordinated copper(I) complexes. International Journal of Quantum Chemistry, 2002, 86, 100-105.	2.0	14
93	Theoretical Evidence of Persistent Chirality in D3 Homoleptic Hexacoordinate Complexes with Monodentate Ligands. Chemistry - A European Journal, 2003, 9, 1952-1957.	3.3	14
94	Concurrent Symmetries: The Interplay Between Local and Global Molecular Symmetries. Chemistry - A European Journal, 2011, 17, 359-367.	3.3	14
95	Charge density wave and metallic state coexistence in the multiband conductor<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mrow><mml:mi>TTF</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub><mml:mo>[</mml:mo> Physical Review B, 2014, 90, .	3.2	14
96	(BEDT-TTF)2Cu2(CN)3 Spin Liquid: Beyond the Average Structure. Crystals, 2018, 8, 158.	2.2	14
97	Ca0.95Nb3O6: Crystal and Electronic Structure. Journal of Solid State Chemistry, 1993, 105, 27-35.	2.9	13
98	A comparative study on the structure of M2Se and M2I+ (M = Ag, Au) using pseudopotentials and full Ab initio methods. International Journal of Quantum Chemistry, 1994, 52, 1-8.	2.0	13
99	Conformational Analysis of Molecular Machines: Internal Rotation and Enantiomerization in Triptycyl[3]helicene. ChemPhysChem, 2008, 9, 1117-1119.	2.1	13
100	Quantifying the symmetry content of the electronic structure of molecules: molecular orbitals and the wave function. Physical Chemistry Chemical Physics, 2010, 12, 15523.	2.8	13
101	Donorâ€“anion interactions at the charge localization and charge ordering transitions of (TMTTF)₂AsF₆ probed by NEXAFS. Physical Chemistry Chemical Physics, 2015, 17, 19202-19214.	2.8	13
102	Electronic structure, bonding, and properties of copper phosphide, CuP2. Inorganic Chemistry, 1992, 31, 119-124.	4.0	12
103	Narcissistic reaction pathways: an example of Maxwellâ€™s theorem of geometrical optics applied to the intrinsic reaction coordinate model. Theoretical Chemistry Accounts, 2008, 121, 279-288.	1.4	12
104	The metallic transport of (TMTSF)₂X organic conductors close to the superconducting phase. Journal of Physics Condensed Matter, 2011, 23, 345702.	1.8	12
105	Theoretical justification of stable ferromagnetism in ferroelectric BiFeO3 by first-principles. Computational Materials Science, 2019, 164, 66-73.	3.0	12
106	Structure of the non-polar (101Ì„0) surfaces of AlN and Î±-SiC: a periodic Hartree-Fock study. Surface Science, 1996, 355, 167-176.	1.9	11
107	Syntheses, Crystal Structures, Transport Properties and First-Principles Electronic Structure Study of the (tTTF)₂X (X = Br, I) Low-Dimensional Antiferromagnets. Inorganic Chemistry, 2011, 50, 4171-4181.	4.0	11
108	Polarization dependence of angle-resolved photoemission with submicron spatial resolution reveals emerging one-dimensionality of electrons in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>NbSe</mml:mi><mml:mn>3</mml:mn></mml:msub></m Physical Review B, 2019, 99, .	3.2	11

#	Article	IF	Citations
109	Continuous symmetry measures of irreducible representations: application to molecular orbitals. Physical Chemistry Chemical Physics, 2012, 14, 11816.	2.8	10
110	Electronic engineering of a tetrathiafulvalene charge-transfer salt via reduced symmetry induced by combined substituents. Physical Chemistry Chemical Physics, 2019, 21, 22639-22646.	2.8	10
111	Combining Chirality and Hydrogen Bonding in Methylated Ethylenedithio-Tetrathiafulvalene Primary Diamide Precursors and Radical Cation Salts. Crystal Growth and Design, 2020, 20, 2516-2526.	3.0	10
112	Conducting chiral nickel(ii) bis(dithiolene) complexes: structural and electron transport modulation with the charge and the number of stereogenic centres. Journal of Materials Chemistry C, 2021, 9, 4119-4140.	5.5	10
113	Metal-ceramic adhesion: band structure calculations on transition-metal-AlN interfaces. Surface Science, 1994, 314, 114-128.	1.9	9
114	Electronic Structure and Magnetic Properties of Potassium Ozonide KO3. Inorganic Chemistry, 2009, 48, 5938-5945.	4.0	9
115	Energy transfer, structural and luminescent properties of the color tunable phosphor Y2WO6:Sm3+. Journal of Alloys and Compounds, 2020, 835, 155381.	5.5	9
116	Magnetic exchange interactions in one-dimensional copper(II) compounds. Chemistry of Materials, 1990, 2, 723-728.	6.7	8
117	Theoretical study of bonding and electrical conductivity in compounds with the NbAs2 structure. Inorganic Chemistry, 1992, 31, 3007-3010.	4.0	8
118	Electronic Structure, Bonding, and Electrical Properties of MoNiP8. Inorganic Chemistry, 1996, 35, 4683-4689.	4.0	8
119	Abinitiostudy of AlN and Î±-SiC (112Â¯0) surface relaxation. Physical Review B, 1996, 53, 4933-4938.	3.2	8
120	Structure and bonding in late transition metal dinuclear complexes with local trigonal planar geometries. Dalton Transactions RSC, 2002, , 2235-2243.	2.3	8
121	Quantitative vs. qualitative approaches to the electronic structure of solids. Journal of Solid State Chemistry, 2003, 176, 375-389.	2.9	8
122	Electronic Structure of the K3Bi2Metallic Phase. Inorganic Chemistry, 2005, 44, 1644-1646.	4.0	8
123	A Continuous Symmetry Analysis of Chemical Bonding. Chemistry - A European Journal, 2011, 17, 6129-6141.	3.3	8
124	Structural Stability of Quaternary ACuFeS₂ (A = Li, K) Phases: A Computational Approach. Inorganic Chemistry, 2012, 51, 362-369.	4.0	8
125	Pseudo-symmetry Analysis of the d-block Molecular Orbitals in Four-Coordinate Complexes. Inorganic Chemistry, 2013, 52, 6510-6519.	4.0	8
126	A fullereneâ€“carbene adduct as a crystalline molecular rotor: remarkable behavior of a spherically-shaped rotator. Physical Chemistry Chemical Physics, 2014, 16, 12980-12986.	2.8	8

#	Article	IF	Citations
127	Câ€“HÂ·Â·Â·BF2O2 Interactions in Crystals: A Case for Boron Hydrogen Bonding?. Crystal Growth and Design, 2014, 14, 3700-3703.	3.0	8
128	Exploring the Electronic Structure of an Organic Semiconductor Based on a Compactly Fused Electron Donorâ€“Acceptor Molecule. ChemPhysChem, 2015, 16, 1361-1365.	2.1	8
129	Charge transfer and 2k_Fvs. 4k_Finstabilities in the NMP-TCNQ molecular metal and (NMP)_x(Phen)_{1â^'x}TCNQ solid solutions. Europhysics Letters, 2016, 113, 27006.	2.0	8
130	Engineering Polar Oxynitrides: Hexagonal Perovskite BaWON₂. Angewandte Chemie - International Edition, 2020, 59, 18395-18399.	13.8	8
131	Heterodox Bonding Effects between Transition Metal Atoms. , 1995, , 241-255.		8
132	Skutterudite vs. ReO3 structures for MX3 solids: electronic requirementsâ€Šâ€¡. Journal of the Chemical Society Dalton Transactions, 1998, , 1195-1200.	1.1	7
133	Electronic Structure of Li2Ga and Li9Al4, Two Solids Containing Infinite and Uniform Zigzag Chains. Inorganic Chemistry, 2005, 44, 374-381.	4.0	7
134	Electronic Structure and Spin Exchange Interactions in Na2V3O7: a Vanadium(IV) Oxide Nanotubular Phase. Inorganic Chemistry, 2009, 48, 5779-5789.	4.0	7
135	Pseudosymmetry analysis of molecular orbitals. Journal of Computational Chemistry, 2013, 34, 1321-1331.	3.3	7
136	Crystallization Induced Enhanced Emission in Two New Zn(II) and Cd(II) Supramolecular Coordination Complexes with the 1-(3,4-Dimethylphenyl)-5-Methyl-1H-1,2,3-Triazole-4-Carboxylate Ligand. Polymers, 2020, 12, 1756.	4.5	7
137	Angular Bond Flexibility and Closed-Shell Metal-Metal Interaction in Polymetal Copper(I), Silver(I) and Gold(I) Iodide Complexes. A Quantum Chemical Study.. Acta Chemica Scandinavica, 1998, 52, 718-727.	0.7	7
138	Crystal Structure and Coexistence of Localized and Delocalized Electrons in Nb12O29. Journal of Solid State Chemistry, 2000, 149, 176-179.	2.9	6
139	Electronic Structure of the A₈Tr₁₁ (A = K, Rb, Cs; Tr = Ga, In, Tl) Zintl Phases: Possible Chemical Reasons Behind Their Activated versus Non Activated Conductivity. Inorganic Chemistry, 2009, 48, 9792-9799.	4.0	6
140	First-principles study of the interaction between paramagnetic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mtext>V</mml:mtext><mml:mrow><mml:mn>4</mml:mn><mml:mo>+</mml:mo></r through formally magnetically inactive<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>VO</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:msu	3.2	6
141	Near-Edge X-ray Absorption Fine Structure Investigation of the Quasi-One-Dimensional Organic Conductor (TMTSF)₂PF₆. Journal of Physical Chemistry A, 2016, 120, 8574-8583.	2.5	6
142	Electronic structure and properties of hexagonal wurtzite-type SiC. International Journal of Quantum Chemistry, 1994, 52, 365-373.	2.0	5
143	Revisiting the foundations of symmetry operation measures for electronic wavefunctions. Chemical Physics Letters, 2011, 511, 486-490.	2.6	5
144	Effects of Temperature on the Shape and Symmetry of Molecules and Solids. Chemistry - A European Journal, 2019, 25, 673-691.	3.3	5

#	Article	IF	Citations
145	Charge Delocalization, Oxidation States, and Silver Mobility in the Mixed Silverâ€“Copper Oxide AgCuO₂. Inorganic Chemistry, 2019, 58, 7026-7035.	4.0	5
146	Electronic Structure and Symmetry in Conjugated Ï€â€Electron Systems. Chemistry - A European Journal, 2011, 17, 14896-14906.	3.3	4
147	Optical Properties of 4-Bromobenzaldehyde Derivatives in Chloroform Solution. Journal of Physical Chemistry A, 2014, 118, 6914-6921.	2.5	4
148	Mixed-valence gold bis(diselenolene) complex turning metallic under pressure. Journal of Materials Chemistry C, 2021, 9, 12291-12302.	5.5	4
149	Monte Carlo study of lactone formation kinetics. Journal of Molecular Structure, 1990, 239, 193-203.	3.6	3
150	Theoretical study of transition-metal adhesion on doped alumina. Chemistry of Materials, 1993, 5, 465-471.	6.7	3
151	Teâ€¦Te Interlayer Interactions, Te â†' Metal Electron Transfer and Electrical Conductivity in the MMâ€²Te5 Phases (M = Nb, Mâ€² = Ni, Pd; M = Ta, Mâ€² = Ni, Pt). European Journal of Inorganic Chemistry, 1999, 1999, 1701-1706.	2.0	3
152	Uniform linear chains of group 11 atoms: do they have a bias towards a Peierls distortion?. Theoretical Chemistry Accounts, 2009, 123, 85-92.	1.4	3
153	A push-pull organic dye with a quinoidal thiophene linker: Photophysical properties and solvent effects. Chemical Physics Letters, 2016, 663, 45-50.	2.6	3
154	Fermi surface properties of the bifunctional organic metal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î¹</mml:mi><mml:mtext>â^'</mml:mtext><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:msub><mml:mrow><mml:mo>(</mml:mo><mml:mi>CN</mml:mi><mml:mo>)</mml:mo></mml:mrow> Physical Review B, 2019, 99, .	3.2	3
155	Electronic, structural, and optical properties of Y2WO6, a host material for inorganic phosphors. Journal of Alloys and Compounds, 2020, 819, 152958.	5.5	3
156	Intermolecular Resonance Correlates Electron Pairs Down a Supermolecular Chain: Antiferromagnetism in K-Doped p-Terphenyl. Journal of the American Chemical Society, 2020, 142, 20624-20630.	13.7	3
157	A Monte Carlo study of the benzene effect on the dipole moment of 1,2-dichloroethane. Chemical Physics Letters, 1989, 156, 525-532.	2.6	2
158	Metal-ceramic interface adhesion: band structure calculations on platinum-nickel(II) oxide couples. Chemistry of Materials, 1993, 5, 459-464.	6.7	2
159	The staging influence on the electronic structure and transport of superconducting sodium-doped hafnium nitride chloride. Journal of Materials Chemistry, 2007, 17, 4362.	6.7	2
160	Hostâ^'Guest Interactions, Uniform vs Fragmented Linear Atom Chains and Likeliness of Peierls Distortions in the (Ca7N4)[Mx] (M = Ag, Ga, In) Phases. Inorganic Chemistry, 2009, 48, 2919-2931.	4.0	2
161	Copper mobility in CuFeS2, a layered trigonal phase obtained from LiCuFeS2. Zeitschrift FÃ¼r Kristallographie, 2010, 225, .	1.1	2
162	Electronic Structure of the Two-Leg Spin Ladder (C5H12N)2CuBr4. Inorganic Chemistry, 2011, 50, 6399-6401.	4.0	2

#	Article	IF	Citations
163	Analyzing the electronic structure of molecules using continuous symmetry measures. International Journal of Quantum Chemistry, 2013, 113, 1814-1820.	2.0	2
164	Engineering a light-driven cyanine based molecular rotor to enhance the sensitivity towards a viscous medium. Materials Advances, 2021, 2, 4804-4813.	5.4	2
165	MnTa₂N₄: A Ternary Nitride Spinel with a Strong Magnetic Frustration. Chemistry of Materials, 2022, 34, 6098-6107.	6.7	2
166	Monte Carlo simulation of 1,2-dichloroethane in dilute benzene solution. Computational and Theoretical Chemistry, 1988, 181, 345-352.	1.5	1
167	Electronic structure calculations and X-ray emission spectra of some metal phosphides. Solid State Communications, 1992, 83, 447-450.	1.9	1
168	Room-Temperature Synthesis and Crystal, Magnetic, and Electronic Structure of the First Silver Copper Oxide.. ChemInform, 2003, 34, no.	0.0	1
169	Factors affecting the magnetic coupling in Sr2V3O9 type oxides: As for V substitution in the VO4 tetrahedra and nature of the cation. Dalton Transactions, 2013, 42, 15555.	3.3	1
170	Assessment of Functionals for First-Principle Studies of the Structural and Electronic Properties ofÎ´-Bi2O3. Advances in Condensed Matter Physics, 2015, 2015, 1-9.	1.1	1
171	Conformational analysis of enantiomerization coupled to internal rotation in triptycyl-n-helicenes. Physical Chemistry Chemical Physics, 2019, 21, 11395-11404.	2.8	1
172	New insights into the structural properties of Îº-(BEDT-TTF)₂Ag₂(CN)₃spin liquid. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 581-590.	1.1	1
173	Weak localization competes with the quantum oscillations in a natural electronic superlattice: The case of <mml:math		

#	Article	IF	Citations
181	Fermi surface and effect of high magnetic fields on the metal-semimetal Peierls-like transition of (TSeT)2Cl. Low Temperature Physics, 2014, 40, 307-310.	0.6	0
182	Metal-charge density wave coexistence in TTF[Ni(dmit)2]2. Physica B: Condensed Matter, 2015, 460, 147-150.	2.7	0
183	Electronic structure of the Î±-(BEDT-TTF)2I3 surface by photoelectron spectroscopy. European Physical Journal B, 2019, 92, 1.	1.5	0
184	Magneto-Structural Correlations in Trinuclear Cu(II) Complexes: A Density Functional Study. , 2003, , 191-200.		0