# Pere Alemany

List of Publications by Year
in descending order

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| 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 | MnTa<sub>2</sub>N<sub>4</sub>: A Ternary Nitride Spinel with a Strong Magnetic Frustration. Chemistry of Materials, 2022, 34, 6098-6107. | 6.7 | 2 |
| 2 | 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 |
| 3 | Rich Polymorphism of Layered NbS<sub>3</sub>. Chemistry of Materials, 2021, 33, 5449-5463. | 6.7 | 18 |
| 4 | Mixed-valence gold bis(diselenolene) complex turning metallic under pressure. Journal of Materials Chemistry C, 2021, 9, 12291-12302. | 5.5 | 4 |
| 5 | 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 |
| 6 | Electronic, structural, and optical properties of Y2WO6, a host material for inorganic phosphors. Journal of Alloys and Compounds, 2020, 819, 152958. | 5.5 | 3 |
| 7 | Engineering Polar Oxynitrides: Hexagonal Perovskite BaWON<sub>2</sub>. Angewandte Chemie - International Edition, 2020, 59, 18395-18399. | 13.8 | 8 |
| 8 | 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 |
| 9 | In Search of Chiral Molecular Superconductors: Îºâ€[(S,S)â€DMâ€BEDTâ€TTF]<sub>2</sub>ClO<sub>4</sub> Revisited. Advanced Materials, 2020, 32, e2002811. | 21.0 | 19 |
| 10 | 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 |
| 11 | New insights into the structural properties of Îº-(BEDT-TTF)<sub>2</sub>Ag<sub>2</sub>(CN)<sub>3</sub>spin liquid. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 581-590. | 1.1 | 1 |
| 12 | Weak localization competes with the quantum oscillations in a natural electronic superlattice: The case of <mml:math | | |

| # | Article | IF | Citations |
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| 19 | Charge Delocalization, Oxidation States, and Silver Mobility in the Mixed Silverâ€“Copper Oxide AgCuO<sub>2</sub>. Inorganic Chemistry, 2019, 58, 7026-7035. | 4.0 | 5 |
| 20 | Fermi surface properties of the bifunctional organic metal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î²</mml:mi><mml:mtext>â˜’</mml:mtext><mml:msub><r mathvariant="normal">N</mml:mi><mml:msub><mml:mrow><mml:mo>(</mml:mo><mml:mi>CN</mml:mi><mml:mo>)</mml:mo></mml:mo></ Physical Review B, 2019, 99, . | 3.2 | 3 |
| 21 | Electronic structure of the Î±-(BEDT-TTF)2I3 surface by photoelectron spectroscopy. European Physical Journal B, 2019, 92, 1. | 1.5 | 0 |
| 22 | Theoretical justification of stable ferromagnetism in ferroelectric BiFeO3 by first-principles. Computational Materials Science, 2019, 164, 66-73. | 3.0 | 12 |
| 23 | 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></ Physical Review B, 2019, 99, . | 3.2 | 11 |
| 24 | 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 |
| 25 | 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 |
| 26 | 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 |
| 27 | (BEDT-TTF)2Cu2(CN)3 Spin Liquid: Beyond the Average Structure. Crystals, 2018, 8, 158. | 2.2 | 14 |
| 28 | Donorâ€“anion interactions in quarter-filled low-dimensional organic conductors. Materials Horizons, 2018, 5, 590-640. | 12.2 | 47 |
| 29 | â€˜Aggregation induced emissionâ€™ active iridium(iii) complexes with applications in mitochondrial staining. RSC Advances, 2017, 7, 5642-5648. | 3.6 | 31 |
| 30 | Structural properties, Juddâ€“Ofelt calculations, and near infrared to visible photon up-conversion in Er<sup>3+</sup>/Yb<sup>3+</sup> doped BaTiO<sub>3</sub> phosphors under excitation at 1500 nm. RSC Advances, 2017, 7, 10529-10538. | 3.6 | 25 |
| 31 | Dual emission and multi-stimuli-response in iridium(<scp>iii</scp>) complexes with aggregation-induced enhanced emission: applications for quantitative CO<sub>2</sub> detection. Journal of Materials Chemistry C, 2017, 5, 7784-7798. | 5.5 | 31 |
| 32 | 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 |
| 33 | 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 |
| 34 | 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 |
| 35 | Near-Edge X-ray Absorption Fine Structure Investigation of the Quasi-One-Dimensional Organic Conductor (TMTSF)<sub>2</sub>PF<sub>6</sub>. Journal of Physical Chemistry A, 2016, 120, 8574-8583. | 2.5 | 6 |
| 36 | Exploring the Origin of â€œAggregation Induced Emissionâ€•Activity and â€œCrystallization Induced Emissionâ€•in Organometallic Iridium(III) Cationic Complexes: Influence of Counterions. Crystal Growth and Design, 2016, 16, 5738-5752. | 3.0 | 27 |

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| 37 | Charge transfer and 2k<sub>F</sub>vs. 4k<sub>F</sub>instabilities in the NMP-TCNQ molecular metal and (NMP)<sub>x</sub>(Phen)<sub>1â^'x</sub>TCNQ solid solutions. Europhysics Letters, 2016, 113, 27006. | 2.0 | 8 |
| 38 | 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 |
| 39 | Structural and electronic control of the metal to insulator transition and local orderings in theÎ¸-(BEDT-TTF)<sub>2</sub>X organic conductors. Journal of Physics Condensed Matter, 2015, 27, 465702. | 1.8 | 15 |
| 40 | 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 |
| 41 | Donorâ€“anion interactions at the charge localization and charge ordering transitions of (TMTTF)<sub>2</sub>AsF<sub>6</sub> probed by NEXAFS. Physical Chemistry Chemical Physics, 2015, 17, 19202-19214. | 2.8 | 13 |
| 42 | Metal-charge density wave coexistence in TTF[Ni(dmit)2]2. Physica B: Condensed Matter, 2015, 460, 147-150. | 2.7 | 0 |
| 43 | Electronic Structure and Magnetic Properties of CuFeS<sub>2</sub>. Inorganic Chemistry, 2015, 54, 4840-4849. | 4.0 | 69 |
| 44 | 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 |
| 45 | Stereochemistry of Complexes with Double and Triple Metalâ€“Ligand Bonds: A Continuous Shape Measures Analysis. Inorganic Chemistry, 2014, 53, 12151-12163. | 4.0 | 17 |
| 46 | 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 |
| 47 | 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>[</mml:mn> Physical Review B, 2014, 90, . | 3.2 | 14 |
| 48 | 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 |
| 49 | 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 |
| 50 | Nature of Holes, Oxidation States, and Hypervalency in Covellite (CuS). Inorganic Chemistry, 2014, 53, 12402-12406. | 4.0 | 68 |
| 51 | 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 |
| 52 | Optical Properties of 4-Bromobenzaldehyde Derivatives in Chloroform Solution. Journal of Physical Chemistry A, 2014, 118, 6914-6921. | 2.5 | 4 |
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| 54 | Distortions of Ï€â€Coordinated Arenes with Anionic Character. Chemistry - A European Journal, 2014, 20, 14674-14689. | 3.3 | 16 |

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| 55 | [illegible] 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 ETQq1 1 0.784314 xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>ClO</mml:mtext><mml:mn>4</mml:mn></mml:msub | | |

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| 73 | Symmetry measures of the electron density. Journal of Computational Chemistry, 2010, 31, 2389-2404. | 3.3 | 19 |
| 74 | Copper mobility in CuFeS2, a layered trigonal phase obtained from LiCuFeS2. Zeitschrift FÃ¼r Kristallographie, 2010, 225, . | 1.1 | 2 |
| 75 | 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></mml:mrow></mml:msup></mml:mrow></mml:math> 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:msub></mml:mrow></mml:math> | 3.2 | 6 |
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| 77 | 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 |
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| 79 | Electronic Structure and Spin Exchange Interactions in Na2V3O7: a Vanadium(IV) Oxide Nanotubular Phase. Inorganic Chemistry, 2009, 48, 5779-5789. | 4.0 | 7 |
| 80 | Electronic Structure of the A<sub>8</sub>Tr<sub>11</sub> (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 |
| 81 | 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 |
| 82 | 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 |
| 83 | Conformational Analysis of Molecular Machines: Internal Rotation and Enantiomerization in Triptycyl[3]helicene. ChemPhysChem, 2008, 9, 1117-1119. | 2.1 | 13 |
| 84 | Symmetry operation measures. Journal of Computational Chemistry, 2008, 29, 190-197. | 3.3 | 55 |
| 85 | 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 |
| 86 | Analytical methods for calculating Continuous Symmetry Measures and the Chirality Measure. Journal of Computational Chemistry, 2008, 29, 2712-2721. | 3.3 | 89 |
| 87 | Molecules and crystals with both icosahedral and cubic symmetry. Chemical Communications, 2008, , 2717. | 4.1 | 43 |
| 88 | 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 |
| 89 | Reply to Comment on â€œDistortions in Octahedrally Coordinated d0Transition Metal Oxides:Â A Continuous Symmetry Measures Approachâ€• Chemistry of Materials, 2007, 19, 1200-1200. | 6.7 | 0 |
| 90 | Density functional study of magnetostructural correlations in cubane complexes containing the Cu4O4core. Journal of Materials Chemistry, 2006, 16, 2729-2735. | 6.7 | 107 |

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| 92 | Distortions in Octahedrally Coordinated d0Transition Metal Oxides:Â A Continuous Symmetry Measures Approach. Chemistry of Materials, 2006, 18, 3176-3183. | 6.7 | 326 |
| 93 | 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 |
| 94 | 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 |
| 95 | 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 |
| 96 | Shape maps and polyhedral interconversion paths in transition metal chemistry. Coordination Chemistry Reviews, 2005, 249, 1693-1708. | 18.8 | 889 |
| 97 | Local Aromaticity of [n]Acenes, [n]Phenacenes, and [n]Helicenes (n = 1â^'9). Journal of Organic Chemistry, 2005, 70, 2509-2521. | 3.2 | 195 |
| 98 | The Rich Stereochemistry of Eight-Vertex Polyhedra: A Continuous Shape Measures Study. Chemistry - A European Journal, 2005, 11, 1479-1494. | 3.3 | 729 |
| 99 | Electronic Structure of Li2Ga and Li9Al4 Two Solids Containing Infinite and Uniform Zigzag Chains.. ChemInform, 2005, 36, no. | 0.0 | 0 |
| 100 | Electron Structure of the K3Bi2 Metallic Phase. ChemInform, 2005, 36, no. | 0.0 | 0 |
| 101 | Continuous Chirality Measures in Transition Metal Chemistry. ChemInform, 2005, 36, no. | 0.0 | 0 |
| 102 | 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 |
| 103 | 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 |
| 104 | Electronic Structure of Li2Ga and Li9Al4, Two Solids Containing Infinite and Uniform Zigzag Chains. Inorganic Chemistry, 2005, 44, 374-381. | 4.0 | 7 |
| 105 | Electronic Structure of the K3Bi2Metallic Phase. Inorganic Chemistry, 2005, 44, 1644-1646. | 4.0 | 8 |
| 106 | Continuous chirality measures in transition metal chemistry. Chemical Society Reviews, 2005, 34, 313. | 38.1 | 98 |
| 107 | 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 |
| 108 | Mapping the Stereochemistry and Symmetry of Tetracoordinate Transition-Metal Complexes. Chemistry - A European Journal, 2004, 10, 190-207. | 3.3 | 175 |

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| 109 | Minimal Distortion Pathways in Polyhedral Rearrangements. Journal of the American Chemical Society, 2004, 126, 1755-1763. | 13.7 | 362 |
| 110 | Magneto-Structural Correlations in Trinuclear Cu(II) Complexes: A Density Functional Study. Monatshefte FÃ¼r Chemie, 2003, 134, 307-316. | 1.8 | 25 |
| 111 | About the calculation of exchange coupling constants in polynuclear transition metal complexes. Journal of Computational Chemistry, 2003, 24, 982-989. | 3.3 | 472 |
| 112 | Room-Temperature Synthesis and Crystal, Magnetic, and Electronic Structure of the First Silver Copper Oxide.. ChemInform, 2003, 34, no. | 0.0 | 1 |
| 113 | Theoretical Evidence of Persistent Chirality in D3 Homoleptic Hexacoordinate Complexes with Monodentate Ligands. Chemistry - A European Journal, 2003, 9, 1952-1957. | 3.3 | 14 |
| 114 | Shape and Symmetry of Heptacoordinate Transition-Metal Complexes: Structural Trends. Chemistry - A European Journal, 2003, 9, 1281-1295. | 3.3 | 225 |
| 115 | Quantitative vs. qualitative approaches to the electronic structure of solids. Journal of Solid State Chemistry, 2003, 176, 375-389. | 2.9 | 8 |
| 116 | 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 |
| 117 | Magneto-Structural Correlations in Trinuclear Cu(II) Complexes: A Density Functional Study. , 2003, , 191-200. | | 0 |
| 118 | Exchange Coupling in Halo-Bridged Dinuclear Cu(II) Compounds:Â A Density Functional Study. Inorganic Chemistry, 2002, 41, 3769-3778. | 4.0 | 118 |
| 119 | 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 |
| 120 | Room-Temperature Synthesis and Crystal, Magnetic, and Electronic Structure of the First Silver Copper Oxide. Inorganic Chemistry, 2002, 41, 6604-6613. | 4.0 | 44 |
| 121 | Structure and bonding in late transition metal dinuclear complexes with local trigonal planar geometries. Dalton Transactions RSC, 2002, , 2235-2243. | 2.3 | 8 |
| 122 | Ligand effects and dimer formation in dicoordinated copper(I) complexes. International Journal of Quantum Chemistry, 2002, 86, 100-105. | 2.0 | 14 |
| 123 | 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 |
| 124 | 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 |
| 125 | Density functional study of the exchange coupling in distorted cubane complexes containing the Cu4O4 core. Polyhedron, 2001, 20, 1323-1327. | 2.2 | 90 |
| 126 | Exchange Coupling in Carboxylato-Bridged Dinuclear Copper(II) Compounds: A Density Functional Study. Chemistry - A European Journal, 2001, 7, 627-637. | 3.3 | 325 |

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| 128 | Crystal Structure and Coexistence of Localized and Delocalized Electrons in Nb12O29. Journal of Solid State Chemistry, 2000, 149, 176-179. | 2.9 | 6 |
| 129 | Theoretical approach to the magnetostructural correlations in the spin-Peierls compoundCuGeO3. Physical Review B, 2000, 61, 54-57. | 3.2 | 16 |
| 130 | The coloring problem in Ba2Cu3VS6â€Šâ€. Dalton Transactions RSC, 2000, , 1009-1011. | 2.3 | 0 |
| 131 | Through-Ring Bonding in Edge Sharing Dimers of Octahedral Complexes. Inorganic Chemistry, 2000, 39, 3166-3175. | 4.0 | 31 |
| 132 | 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 |
| 133 | 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 |
| 134 | Tetrahedral d0 and d10 transition metal ions sharing edges in the solid state: electronic structure and bonding. Journal of the Chemical Society Dalton Transactions, 1999, , 1235-1240. | 1.1 | 0 |
| 135 | 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 |
| 136 | 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 |
| 137 | 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 |
| 138 | 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 |
| 139 | Chemical Transport Synthesis, Electrochemical Behavior, and Electronic Structure of Superconducting Zirconium and Hafnium Nitride Halides. Inorganic Chemistry, 1999, 38, 4530-4538. | 4.0 | 25 |
| 140 | Electronic Structure and Bonding in Tricoordinate Amido Complexes of Transition Metals. Inorganic Chemistry, 1999, 38, 707-715. | 4.0 | 16 |
| 141 | Theoretical search for new ferromagnetically coupled transition metal complexes. Chemical Communications, 1998, , 2767-2768. | 4.1 | 62 |
| 142 | Exchange Coupling in Oxalato-Bridged Copper(II) Binuclear Compounds: A Density Functional Study. Chemistry - A European Journal, 1998, 4, 476-484. | 3.3 | 197 |
| 143 | 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 |
| 144 | Skutterudite vs. ReO3 structures for MX3 solids: electronic requirementsâ€Šâ€¡. Journal of the Chemical Society Dalton Transactions, 1998, , 1195-1200. | 1.1 | 7 |

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| 146 | 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 |
| 147 | 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 |
| 148 | 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 |
| 149 | Electronic Structure and Dynamic Properties of Solid Alkali Cyanides. Journal of Physical Chemistry A, 1997, 101, 1393-1399. | 2.5 | 14 |
| 150 | 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 |
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| 152 | 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 |
| 153 | Electronic structure and properties ofCu2O. Physical Review B, 1997, 56, 7189-7196. | 3.2 | 146 |
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| 156 | 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 |
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