# Ramiro Arratia-Perez

## List of Publications by Citations



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| 166 papers | 2,388 citations | 25 h-index | 37 g-index |
| 169 ext. papers | 2,633 ext. citations | 3.4 avg, IF | 5.08 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 166 | The Re6Se8Cl64− and Re6Se8I64− cluster ions: Another example of luminescent clusters?. *Journal of Chemical Physics*, **1999**, 111, 168-172 | 3.9 | 72 |
| 165 | The hexanuclear rhenium cluster ions Re6S8X64− (X=Cl, Br, I): Are these clusters luminescent?. *Journal of Chemical Physics*, **1999**, 110, 2529-2532 | 3.9 | 70 |
| 164 | Enhancement of the Catalytic Activity of Fe Phthalocyanine for the Reduction of O2 Anchored to Au(111) via Conjugated Self-Assembled Monolayers of Aromatic Thiols As Compared to Cu Phthalocyanine. *Journal of Physical Chemistry C*, **2012**, 116, 15329-15341 | 3.8 | 63 |
| 163 | Quantum Dynamical Simulations as a Tool for Predicting Photoinjection Mechanisms in Dye-Sensitized TiO2 Solar Cells. *Journal of Physical Chemistry Letters*, **2012**, 3, 2548-55 | 6.4 | 55 |
| 162 | Electronic structure and molecular properties of the [Mo6X8L6]2− (X = Cl, Br, I; L = F, Cl, Br, I clusters. *Chemical Physics Letters*, **2008**, 460, 438-441 | 2.5 | 52 |
| 161 | Intramolecular and lateral intermolecular hole transfer at the sensitized TiO2 interface. *Journal of the American Chemical Society*, **2014**, 136, 1034-46 | 16.4 | 51 |
| 160 | Theoretical study of sensitizer candidates for dye-sensitized solar cells: peripheral substituted dizinc pyrazinoporphyrazine-phthalocyanine complexes. *Journal of Physical Chemistry A*, **2013**, 117, 430-8 | 2.8 | 45 |
| 159 | The paramagnetic and luminescent [Re6Se8I6]3− cluster. Its potential use as an antitumoral and biomarker agent. *New Journal of Chemistry*, **2012**, 36, 927 | 3.6 | 42 |
| 158 | Theoretical Method for an Accurate Elucidation of Energy Transfer Pathways in Europium(III) Complexes with Dipyridophenazine (dppz) Ligand: One More Step in the Study of the Molecular Antenna Effect. *Inorganic Chemistry*, **2017**, 56, 9200-9208 | 5.1 | 40 |
| 157 | Calculated electronic structure of Au13 clusters. *Physical Review B*, **1989**, 39, 3005-3009 | 3.3 | 40 |
| 156 | Tellurium(0) as a ligand: synthesis and characterization of 2-pyridyltellurolates of platinum(II) and structures of [Pt{2-Te-3-(R)C5H3N}2Te(PR'3)] (R = H or Me). *Inorganic Chemistry*, **2010**, 49, 4179-85 | 5.1 | 38 |
| 155 | A TD-DFT basis set and density functional assessment for the calculation of electronic excitation energies of fluorene. *International Journal of Quantum Chemistry*, **2012**, 112, 3434-3438 | 2.1 | 37 |
| 154 | Oxidative perhydroxylation of [closo-B12H12]2- to the stable inorganic cluster redox system [B12(OH)12](2-/*-): experiment and theory. *Chemistry - A European Journal*, **2010**, 16, 11242-5 | 4.8 | 36 |
| 153 | Calculated paramagnetic resonance parameters (g,Ahfi) of the Re6S8Br63− Re6S8I63− and Re6Se8I63− cluster ions. *Journal of Chemical Physics*, **2003**, 118, 7425 | 3.9 | 36 |
| 152 | Dirac scattered-wave calculations on an icosahedral Au13 cluster. *Physical Review B*, **1987**, 35, 3790-3798 | 3.3 | 35 |
| 151 | Spin-orbit effects on a gold-based superatom: a relativistic Jellium model. *Physical Chemistry Chemical Physics*, **2012**, 14, 1408-11 | 3.6 | 33 |
| 150 | Spin-orbit effects on electronic delocalization. Aromaticity in a discrete square tetrapalladium sandwich complex. *Journal of Chemical Physics*, **2010**, 132, 164308 | 3.9 | 33 |

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| 149 | Ground state of octahedral platinum hexafluoride. *Physical Review A*, **2008**, 77, | 2.6 | 33 |
| 148 | Spin□orbit effects on the aromaticity of the Re3Cl9 and Re3Br9 clusters. *Chemical Physics Letters*, **2008**, 467, 94-96 | 2.5 | 33 |
| 147 | Reactivity of Dipyridyl Ditellurides with (Diphosphine)Pt0 and 2-Pyridyltellurolates with (Diphosphine)PtCl2 and Isolation of Different Structural Motifs of Platinum(II) Complexes. *Organometallics*, **2012**, 31, 1743-1750 | 3.8 | 32 |
| 146 | Electronic delocalization, energetics, and optical properties of tripalladium ditropylium halides, [Pd(3)(C(7)H(7))(2)X(3)](1-) (X = Cl(-), Br(-), and I(-)). *Journal of Physical Chemistry A*, **2010**, 114, 5217-21 | 2.8 | 30 |
| 145 | Calculated optical and magnetic properties of hexafluorouranate (V) anion: UF- 6. *Journal of Chemical Physics*, **2004**, 121, 7743-7 | 3.9 | 30 |
| 144 | Calculated molecular properties of triangular tribenzo and perfluoro-tribenzo trimercuronin macrocycles. *Journal of Physical Chemistry A*, **2010**, 114, 666-72 | 2.8 | 26 |
| 143 | Study of the structure□bioactivity relationship of three new pyridine Schiff bases: synthesis, spectral characterization, DFT calculations and biological assays. *New Journal of Chemistry*, **2018**, 42, 8851-8863 | 3.6 | 25 |
| 142 | Spin-orbit effects on the aromaticity of the Re3X9(2-) (X = Cl, Br) cluster ions. *Journal of Physical Chemistry A*, **2009**, 113, 1671-3 | 2.8 | 25 |
| 141 | Calculated paramagnetic resonance parameters of the luminescent Re6S8Cl63□cluster ion. *Journal of Chemical Physics*, **2001**, 115, 726-730 | 3.9 | 25 |
| 140 | Luminescent europium(III) and terbium(III) complexes of □diketonate and substituted terpyridine ligands: synthesis, crystal structures and elucidation of energy transfer pathways. *New Journal of Chemistry*, **2019**, 43, 15139-15152 | 3.6 | 24 |
| 139 | The luminescent [Mo6X8(NCS)6]2□(X=Cl, Br, I) clusters?: A computational study based on time-dependent density functional theory including spin□orbit and solvent-polarity effects. *Chemical Physics Letters*, **2008**, 455, 38-41 | 2.5 | 24 |
| 138 | Inside a superatom: the M7q (M=Cu, Ag, q=1+, 0, 1-) case. *ChemPhysChem*, **2010**, 11, 646-50 | 3.2 | 23 |
| 137 | Theoretical insights into the adsorption of neutral, radical and anionic thiophenols on gold(111). *Physical Chemistry Chemical Physics*, **2013**, 15, 20363-70 | 3.6 | 22 |
| 136 | The Synthesis of Stable, Complex Organocesium Tetramic Acids through the Ugi Reaction and Cesium-Carbonate-Promoted Cascades. *Angewandte Chemie - International Edition*, **2015**, 54, 11672-6 | 16.4 | 22 |
| 135 | Bonding nature and electron delocalization of An(COT)2, An = Th, Pa, U. *Journal of Physical Chemistry A*, **2011**, 115, 8997-9003 | 2.8 | 22 |
| 134 | Electronic structure, molecular properties and electronic currents of the luminescent [Au3(CH3NCOCH3)3] cluster. *Chemical Physics Letters*, **2009**, 474, 290-293 | 2.5 | 22 |
| 133 | Theoretical Determination of Energy Transfer Processes and Influence of Symmetry in Lanthanide(III) Complexes: Methodological Considerations. *Inorganic Chemistry*, **2018**, 57, 5120-5132 | 5.1 | 21 |
| 132 | Direct Spectroscopic Evidence for Constituent Heteroatoms Enhancing Charge Recombination at a TiO2□Ruthenium Dye Interface. *Journal of Physical Chemistry C*, **2014**, 118, 17079-17089 | 3.8 | 20 |

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| 131 | Pyridine as axial ligand on the [Mo6Cl8]4+ core switches off luminescence. *Chemical Physics Letters*, **2009**, 475, 232-234 | 2.5 | 20 |
| 130 | Nanostructuring of anodic copper oxides in fluoride-containing ethylene glycol media. *Journal of Electroanalytical Chemistry*, **2017**, 807, 181-186 | 4.1 | 19 |
| 129 | Experimental and theoretical studies of the ancillary ligand (E)-2-((3-amino-pyridin-4-ylimino)-methyl)-4,6-di-tert-butylphenol in the rhenium(I) core. *New Journal of Chemistry*, **2015**, 39, 5725-5734 | 3.6 | 19 |
| 128 | A relativistic study of the electronic and magnetic properties of cerocene and thorocene and its anions. *Journal of Physical Chemistry A*, **2012**, 116, 4170-5 | 2.8 | 19 |
| 127 | [Cp*Ru(s-indacene)RuCp*] and [Cp*Ru(s-indacene)RuCp*]+: Experimental and theoretical findings concerning the electronic structure of neutral and mixed valence organometallic systems. *Polyhedron*, **2010**, 29, 1137-1143 | 2.7 | 19 |
| 126 | Calculated paramagnetic hyperfine structure of pentagonal bipyramid Ag7 cluster. *Journal of Chemical Physics*, **1998**, 108, 5795-5798 | 3.9 | 19 |
| 125 | Bonding in the octahedral Au62+ cluster. *Chemical Physics Letters*, **1986**, 125, 143-148 | 2.5 | 19 |
| 124 | Rare-Earth Metal(II) Aryloxides: Structure, Synthesis, and EPR Spectroscopy of [K(2.2.2-cryptand)][Sc(OC H tBu -2,6-Me-4) ]. *Chemistry - A European Journal*, **2018**, 24, 18059-18067 | 4.8 | 19 |
| 123 | Substituted bidentate and ancillary ligands modulate the bioimaging properties of the classical Re(I) tricarbonyl core with yeasts and bacteria. *New Journal of Chemistry*, **2017**, 41, 2140-2147 | 3.6 | 18 |
| 122 | Electronic Structure and Properties of Berkelium Iodates. *Journal of the American Chemical Society*, **2017**, 139, 13361-13375 | 16.4 | 18 |
| 121 | Geometrically specific imino complexes of the [Re6(μ3-Se)8]2+ core-containing clusters. *Chemistry - A European Journal*, **2011**, 17, 580-7 | 4.8 | 18 |
| 120 | Theoretical and Experimental Study of Bonding and Optical Properties of Self-Assembly Metallophthalocyanines Complexes on a Gold Surface. A Survey of the Substrate−Surface Interaction.. *Journal of Physical Chemistry C*, **2011**, 115, 23512-23518 | 3.8 | 18 |
| 119 | Chromium(III) complexes with terdentate 2,6-bis(azolylmethyl)pyridine ligands: Synthesis, structures and ethylene polymerization behavior. *Journal of Organometallic Chemistry*, **2009**, 694, 2636-2641 | 2.3 | 18 |
| 118 | Relativistic molecular orbital study of the optical and magnetic properties of hexachloro protactinate (IV): PaCl6(2-). *Journal of Chemical Physics*, **2006**, 124, 74321 | 3.9 | 18 |
| 117 | Relativistic electronic structure of an icosahedral Au12Pd cluster. *Chemical Physics Letters*, **1999**, 303, 641-648 | 2.5 | 18 |
| 116 | Coinage Metal Superatomic Cores: Insights into Their Intrinsic Stability and Optical Properties from Relativistic DFT Calculations. *Chemistry - A European Journal*, **2017**, 23, 11330-11337 | 4.8 | 17 |
| 115 | Simulation of natural dyes adsorbed on TiO2 for photovoltaic applications. *Solar Energy*, **2017**, 142, 215-228 | 3.3 | 17 |
| 114 | Quantum relativistic investigation about the coordination and bonding effects of different ligands on uranyl complexes. *Polyhedron*, **2010**, 29, 975-984 | 2.7 | 17 |

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| 113 | Cluster-bound nitriles do not click with organic azides: unexpected formation of imino complexes of the [Re(6)(mu(3)-Se)(8)](2+) core-containing clusters. *Inorganic Chemistry*, **2010**, 49, 380-2 | 5.1 | 16 |
| 112 | Cluster carbonyls of the [Re(6)(mu(3)-Se)(8)](2+) core: synthesis, structural characterization, and computational analysis. *Dalton Transactions*, **2008**, 4247-53 | 4.3 | 16 |
| 111 | The M6S8L6 clusters: an example in cluster and condensed phase chemistry. *Chemical Physics Letters*, **1993**, 213, 547-553 | 2.5 | 16 |
| 110 | Spectral, theoretical characterization and antifungal properties of two phenol derivative Schiff bases with an intramolecular hydrogen bond. *New Journal of Chemistry*, **2015**, 39, 7822-7831 | 3.6 | 15 |
| 109 | Rhenium (I) Complexes as Probes for Prokaryotic and Fungal Cells by Fluorescence Microscopy: Do Ligands Matter?. *Frontiers in Chemistry*, **2019**, 7, 454 | 5 | 15 |
| 108 | Understanding the influence of terminal ligands on the electronic structure and bonding nature in [Re6(□-Q8)](2+) clusters. *Journal of Physical Chemistry A*, **2014**, 118, 11083-9 | 2.8 | 15 |
| 107 | Optical and Magnetic Properties of the Complex Bis(dicyclooctatetraenyl)diuranium. A Theoretical View. *Organometallics*, **2012**, 31, 6297-6304 | 3.8 | 15 |
| 106 | A DFT/TDDFT study of porphyrazines and phthalocyanine oxo-titanium derivatives as potential dyes in solar cells. *International Journal of Quantum Chemistry*, **2011**, 111, 4186-4196 | 2.1 | 15 |
| 105 | Pi-donor/acceptor effect on Lindqvist type polyoxomolibdates because of various multiple-bonded nitrogenous ligands. *Journal of Physical Chemistry A*, **2007**, 111, 6563-7 | 2.8 | 15 |
| 104 | Spin□rbit effects on heavy metal octahedral clusters. *Computational and Theoretical Chemistry*, **1993**, 282, 131-141 | | 15 |
| 103 | Cyclic voltammetry, relativistic DFT calculations and biological test of cytotoxicity in walled-cell models of two classical rhenium (I) tricarbonyl complexes with 5-amine-1,10-phenanthroline. *Chemical Physics Letters*, **2019**, 715, 231-238 | 2.5 | 15 |
| 102 | Substituents role in zinc phthalocyanine derivatives used as dye-sensitized solar cells. A theoretical study using Density Functional Theory. *Chemical Physics Letters*, **2015**, 639, 172-177 | 2.5 | 14 |
| 101 | New Insights into Re3(□Cl)3Cl6 Aromaticity. Evidence of □and □Diatropicity. *Journal of Physical Chemistry Letters*, **2015**, 6, 4326-30 | 6.4 | 14 |
| 100 | Reduction of Au(III) by a □cyclodextrin polymer in acid medium. A stated unattainable reaction. *Carbohydrate Polymers*, **2017**, 175, 530-537 | 10.3 | 14 |
| 99 | Probing the aromaticity of the [(H(t)Ac)3(□-H)6], [(H(t)Th)3(□-H)6],(+), and [(H(t)Pa)3(□-H)6] clusters. *Journal of Chemical Physics*, **2011**, 135, 104506 | 3.9 | 14 |
| 98 | A Dirac molecular orbital study for hexanuclear tungsten cluster structures. *Chemical Physics Letters*, **1997**, 277, 223-226 | 2.5 | 14 |
| 97 | Calculated paramagnetic resonance parameters of a gallium arsenide cluster: Ga2As3. *Journal of Chemical Physics*, **1998**, 109, 3497-3500 | 3.9 | 14 |
| 96 | The role of the [CpM(CO)2](-) chromophore in the optical properties of the [Cp2ThMCp(CO)2](+) complexes, where M = Fe, Ru and Os. A theoretical view. *Dalton Transactions*, **2015**, 44, 20004-10 | 4.3 | 13 |

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| 95 | Interaction of LD14 and TiO2 in dye-sensitized solar-cells (DSSC): A density functional theory study. *Computational and Theoretical Chemistry*, **2015**, 1070, 117-125 | 2 | 13 |
| 94 | Theoretical and experimental characterization of a novel pyridine benzimidazole: suitability for fluorescence staining in cells and antimicrobial properties. *New Journal of Chemistry*, **2016**, 40, 2362-2375 | 3.6 | 13 |
| 93 | Two New Fluorinated Phenol Derivatives Pyridine Schiff Bases: Synthesis, Spectral, Theoretical Characterization, Inclusion in Epichlorohydrin-β-Cyclodextrin Polymer, and Antifungal Effect. *Frontiers in Chemistry*, **2018**, 6, 312 | 5 | 13 |
| 92 | Exploring the geometrical and optical properties of neutral rhenium (I) tricarbonyl complex of 1,10-phenanthroline-5,6-diol using relativistic methods. *Chemical Physics Letters*, **2017**, 685, 354-362 | 2.5 | 13 |
| 91 | Interaction of YD2 and TiO2 in dye-sensitized solar cells (DSSCs): a density functional theory study. *Journal of Molecular Modeling*, **2015**, 21, 226 | 2 | 12 |
| 90 | Atomic force microscopy (AFM) and 3D confocal microscopy as alternative techniques for the morphological characterization of anodic TiO 2 nanoporous layers. *Materials Letters*, **2016**, 165, 67-70 | 3.3 | 12 |
| 89 | A new heterobimetallic manganese–rhodium carbonyl complex derived from partially alkylated s-indacene. *Inorganica Chimica Acta*, **2013**, 394, 132-139 | 2.7 | 12 |
| 88 | Optical and electronic properties of benzopyrylium derivatives. Theoretical-experimental synergy towards novel DSSCs devices. *Dyes and Pigments*, **2019**, 161, 370-381 | 4.6 | 12 |
| 87 | Electrochemical behaviors and relativistic DFT calculations to understand the terminal ligand influence on the [Re6(μ3-Q)8X6]4− clusters. *New Journal of Chemistry*, **2018**, 42, 5471-5478 | 3.6 | 11 |
| 86 | Role of the main adsorption modes in the interaction of the dye [COOH-TPP-Zn(II)] on a periodic TiO2 slab exposing a rutile (110) surface in a dye-sentized solar cell. *RSC Advances*, **2014**, 4, 9639 | 3.7 | 11 |
| 85 | Electronic structure and optical properties calculation of Zn-porphyrin with N-annulated perylene adsorbed on TiO2 model for dye-sensitized solar cell applications: A DFT/TD-DFT study. *Computational Materials Science*, **2017**, 126, 514-527 | 3.2 | 11 |
| 84 | Electronic structure of tungsten hexacarbonyl. *Chemical Physics Letters*, **1984**, 107, 112-116 | 2.5 | 11 |
| 83 | The Synthesis of Stable, Complex Organocesium Tetramic Acids through the Ugi Reaction and Cesium-Carbonate-Promoted Cascades. *Angewandte Chemie*, **2015**, 127, 11838-11842 | 3.6 | 10 |
| 82 | Covalent lanthanide(III) macrocyclic complexes: the bonding nature and optical properties of a promising single antenna molecule. *Physical Chemistry Chemical Physics*, **2014**, 16, 25978-88 | 3.6 | 9 |
| 81 | Photophysical properties of [Cu(binap)2]+ and [Pd(binap)2] complexes: A theoretical study. *Polyhedron*, **2012**, 37, 54-59 | 2.7 | 9 |
| 80 | Substituents effects on two related families of dyes for dye sensitized solar cells: [Ru(4,4′-R,R-2,2′-bpy)(3)]2+ and [Ru(4,4′-COOH-2,2′-bpy)(4,4′-R,R-2,2′-bpy)(2)]2+. *Journal of Physical Chemistry A*, **2012**, 116, 7436-42 | 2.8 | 9 |
| 79 | New bis(azolylcarbonyl)pyridine chromium(III) complexes as initiators for ethylene polymerization. *Inorganica Chimica Acta*, **2011**, 378, 218-223 | 2.7 | 9 |
| 78 | SPIN-ORBIT AND SOLVENT EFFECTS IN THE LUMINESCENT [Re6Q8(NCS)6]4-, Q=S, Se, Te CLUSTERS: MOLECULAR SENSORS AND MOLECULAR DEVICES. *Journal of the Chilean Chemical Society*, **2010**, 55, | 2.5 | 9 |

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| 77 | Relativistic scalar and spin□orbit density functional calculations of the electronic structure, NICS index and ELF function of the [Re2(CO)8(□BiPh)2] and [Re2(CO)8(□BiPh2)2] clusters. *Polyhedron*, **2011**, 30, 846-850 | 2.7 | 9 |
| 76 | Calculated geometry and paramagnetic hyperfine structure of the Cu7 cluster. *Chemical Physics Letters*, **2004**, 397, 408-411 | 2.5 | 9 |
| 75 | Electronic structure of octachloroditungstate(II). *Inorganic Chemistry*, **1984**, 23, 3271-3273 | 5.1 | 9 |
| 74 | Surface on Surface. Survey of the Monolayer Gold□raphene Interaction from Au12 and PAH via Relativistic DFT Calculations. *Journal of Physical Chemistry C*, **2016**, 120, 7358-7364 | 3.8 | 8 |
| 73 | Relativistic effects in bonding and isomerization energy of the superheavy roentgenium (111Rg) cyanide. *Polyhedron*, **2012**, 39, 113-117 | 2.7 | 8 |
| 72 | Antenna effect by organometallic chromophores in bimetallic d-f complexes. *Journal of Physical Chemistry A*, **2013**, 117, 7847-54 | 2.8 | 8 |
| 71 | The origin of phosphorescence in Iridium (III) complexes. The role of relativistic effects. *Chemical Physics Letters*, **2017**, 685, 60-68 | 2.5 | 8 |
| 70 | Exploring the nature of the excitation energies in [Re6(□3-Q8)X6](4-) clusters: a relativistic approach. *Physical Chemistry Chemical Physics*, **2015**, 17, 17611-7 | 3.6 | 8 |
| 69 | Toward the synthetic control of the HOMO-LUMO gap in binuclear systems: insights from density functional calculations. *Inorganic Chemistry*, **2010**, 49, 4175-8 | 5.1 | 8 |
| 68 | DFT study on the electronic structure, energetics and spectral properties of several bis(organohydrazido(2-)) molybdenum complexes containing substituted phosphines and chloro atoms as ancillary ligands. *Computational and Theoretical Chemistry*, **2010**, 957, 126-132 | | 8 |
| 67 | Calculated paramagnetic properties of matrix isolated Au3 cluster. *Chemical Physics Letters*, **1995**, 236, 37-42 | 2.5 | 8 |
| 66 | Spin□orbit effects on RuO4 and OsO4. *Chemical Physics Letters*, **1993**, 203, 409-414 | 2.5 | 8 |
| 65 | Molecular and Electronic Structure, and Hydrolytic Reactivity of a Samarium(II) Crown Ether Complex. *Inorganic Chemistry*, **2019**, 58, 3457-3465 | 5.1 | 8 |
| 64 | DFT studies on coordination models for adsorption essays of Cu(II) and Ni(II) solutions in modified silica gel with iminodiacetic groups. *Chemical Papers*, **2017**, 71, 1019-1030 | 1.9 | 7 |
| 63 | Synthesis, characterization and relativistic DFT studies of fac -Re(CO) 3 (isonicotinic acid) 2 Cl complex. *Chemical Physics Letters*, **2017**, 688, 66-73 | 2.5 | 7 |
| 62 | [M16Ni24(CO)40]4□Coinage Metal Tetrahedral Superatoms as Useful Building Blocks Related to Pyramidal Au20 Clusters (M = Cu, Ag, Au). Electronic and Bonding Properties from Relativistic DFT Calculations. *Journal of Physical Chemistry C*, **2018**, 122, 4723-4730 | 3.8 | 7 |
| 61 | New mono and bimetallic iron complexes derived from partially methylated s-indacene. Evidence of a trinuclear iron s-indacene complex. *Polyhedron*, **2014**, 69, 15-24 | 2.7 | 7 |
| 60 | Spin□orbit effects on the optical and magnetic properties of cerium (III) hexahalides. *Polyhedron*, **2011**, 30, 860-863 | 2.7 | 7 |

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| 59 | Electronic structure and molecular properties of the heptacyanorhenate [Re(CN)7]3- and [Re(CN)7]4- complexes. *Journal of Physical Chemistry A*, **2006**, 110, 1072-7 | 2.8 | 7 |
| 58 | Calculated paramagnetic properties of the acute GaAs2 and obtuse Ga2As clusters. *Journal of Chemical Physics*, **1999**, 110, 10882-10887 | 3.9 | 7 |
| 57 | Catalytic aspects of metallophthalocyanines adsorbed on gold-electrode. Theoretical exploration of the binding nature role. *Physical Chemistry Chemical Physics*, **2016**, 18, 29516-29525 | 3.6 | 7 |
| 56 | Spin-orbit effect into isomerization barrier of small gold Clusters. Oh <-fD2h Fluxionality of the Au62+ cluster Investigated by relativistic methods. *Chemical Physics Letters*, **2017**, 683, 404-407 | 2.5 | 6 |
| 55 | X-ray diffraction and relativistic DFT studies on the molecular biomarker fac-Re(CO)3(4,4?-dimethyl-2,2?-bpy)(E-2-((3-amino-pyridin-4-ylimino)-methyl)-4,6-di-tert-butylphenol)(PF6) *Chemical Papers*, **2017**, 71, 2011-2022 | 1.9 | 6 |
| 54 | Aromatic Lateral Substituents Influence the Excitation Energies of Hexaaza Lanthanide Macrocyclic Complexes: A Wave Function Theory and Density Functional Study. *Journal of Physical Chemistry A*, **2015**, 119, 9931-40 | 2.8 | 6 |
| 53 | Improvement of photovoltaic performance by substituent effect of donor and acceptor structure of TPA-based dye-sensitized solar cells. *Journal of Molecular Modeling*, **2016**, 22, 25 | 2 | 6 |
| 52 | The aromaticity of the [Re3(□X)3X9]3□clusters, X = Cl, Br, I. *Chemical Physics Letters*, **2012**, 545, 50-53 | 2.5 | 6 |
| 51 | Methylation and the system-size effect over the structural, electronic, magnetic (NICS) and reactive properties of pentalene derivatives. *Chemical Physics Letters*, **2012**, 545, 88-94 | 2.5 | 6 |
| 50 | ADSORPTION ESSAYS OF PALLADIUM IN MODIFIED SILICA GEL WITH THIOURONIUM GROUPS: EXPERIMENTAL AND THEORICAL STUDIES. *Journal of the Chilean Chemical Society*, **2011**, 56, 692-696 | 2.5 | 6 |
| 49 | Heterobimetallic Re=Pd complexes bridged by eta(1):eta(5)-Ph(2)PC(5)H(4) ligand. Synthesis, electronic and crystal structure of (CO)(2)(PR(3))(eta(5)-C(5)H(4)PPh(2))Re-PdCl(2), R = Me and OMe. *Dalton Transactions*, **2010**, 39, 6295-301 | 4.3 | 6 |
| 48 | Electronic structure and metal□metal communication in (CpM)2(as-indacene) and (CpM)2(s-indacene) (M = Mn, Fe, Co, Ni) complexes: a DFT investigation. *New Journal of Chemistry*, **2011**, 35, 2136 | 3.6 | 6 |
| 47 | Relativistic calculations of aminotroponiminate complexes containing group 15 (P, As, Sb, Bi) elements. *Polyhedron*, **2011**, 30, 841-845 | 2.7 | 6 |
| 46 | A Dirac molecular orbital study for the tetragonal compression in the RuY6I122□cluster. *Chemical Physics Letters*, **1996**, 255, 217-222 | 2.5 | 6 |
| 45 | Calculated Paramagnetic Hyperfine Structure of the C2v Isomers of Ag3. *The Journal of Physical Chemistry*, **1994**, 98, 5627-5631 | | 6 |
| 44 | Paramagnetic resonance hyperfine structure of hexachloroprotactinate(IV). *Physical Review B*, **1988**, 37, 4893-4899 | 3.3 | 6 |
| 43 | Density functional study on Keggin heteropolyanions containing fifth period main group heteroatoms. *Polyhedron*, **2016**, 117, 478-486 | 2.7 | 6 |
| 42 | Bonding in gold-rare earth [Au2M] (M = Eu, Yb, Lu) ions. A strong covalent gold-lanthanide bond. *Chemical Physics Letters*, **2017**, 683, 421-424 | 2.5 | 5 |

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| 41 | Ab initio calculations of heavy-actinide hexahalide compounds: do these heavy actinides behave like their isoelectronic lanthanide analogues?. *Physical Chemistry Chemical Physics*, **2018**, 20, 4038-4049 | 3.6 | 5 |
| 40 | Theoretical exploration of seleno and tellurophenols as promising alternatives to sulfur ligands for anchoring to gold (111) materials. *RSC Advances*, **2016**, 6, 4458-4468 | 3.7 | 5 |
| 39 | Electronic structure and molecular properties of the octacyanorhenate [Re(CN)8]3− and [Re(CN)8]2− complexes. *Chemical Physics Letters*, **2006**, 422, 89-94 | 2.5 | 5 |
| 38 | A Dirac molecular orbital study for encapsulated heavy transition metals within ytrium cluster iodides. *Chemical Physics Letters*, **1995**, 247, 163-167 | 2.5 | 5 |
| 37 | Geometry, bonding and optical and magnetic properties of copper tricarbonyl: a theoretical study. *The Journal of Physical Chemistry*, **1987**, 91, 5177-5183 | | 5 |
| 36 | Insights into the role of D-A-π-A type pro-aromatic organic dyes with thieno[3,4-b]pyrazine as A acceptor group into dye-sensitized solar-cells. A TD-DFT/periodic DFT study. *International Journal of Quantum Chemistry*, **2020**, 120, e26108 | 2.1 | 5 |
| 35 | The role of zero-field splitting and π-stacking interaction of different nitrogen-donor ligands on the optical properties of luminescent rhenium tricarbonyl complexes. *New Journal of Chemistry*, **2021**, 45, 11192-11201 | 3.6 | 5 |
| 34 | Survey of short and long cuprophilic d10–d10 contacts for tetranuclear copper clusters. Understanding of bonding and ligand role from a planar superatom perspective. *New Journal of Chemistry*, **2018**, 42, 8874-8881 | 3.6 | 4 |
| 33 | Three new types of transition metal carboranylamidinate complexes. *Dalton Transactions*, **2018**, 47, 6666-6671 | 4.5 | 4 |
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