Ramiro Arratia-Perez

List of Publications by Year
in descending order

166 papers	2,795 citations	201658 27 h-index	302107 39 g-index
169 all docs	169 docs citations	169 times ranked	2722 citing authors

#	Article	IF	Citations
1	The Re6Se8Cl64â^' and Re6Se8I64â^' cluster ions: Another example of luminescent clusters?. Journal of Chemical Physics, 1999, 111, 168-172.	3.0	75
2	The hexanuclear rhenium cluster ions Re6S8X64â^' (X=Cl, Br, I): Are these clusters luminescent?. Journal of Chemical Physics, 1999, 110, 2529-2532.	3.0	73
3	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.	3.1	69
4	Quantum Dynamical Simulations as a Tool for Predicting Photoinjection Mechanisms in Dye-Sensitized TiO₂ Solar Cells. Journal of Physical Chemistry Letters, 2012, 3, 2548-2555.	4.6	63
5	Electronic structure and molecular properties of the [Mo6X8L6]2â^'; X=Cl, Br, I; L=F, Cl, Br, I clusters. Chemical Physics Letters, 2008, 460, 438-441.	2.6	58
6	Intramolecular and Lateral Intermolecular Hole Transfer at the Sensitized TiO₂ Interface. Journal of the American Chemical Society, 2014, 136, 1034-1046.	13.7	54
7	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.	4.0	53
8	Theoretical Study of Sensitizer Candidates for Dye-Sensitized Solar Cells: Peripheral Substituted Dizinc Pyrazinoporphyrazineâ€"Phthalocyanine Complexes. Journal of Physical Chemistry A, 2013, 117, 430-438.	2.5	50
9	Calculated electronic structure ofAu13clusters. Physical Review B, 1989, 39, 3005-3009.	3.2	45
10	The paramagnetic and luminescent [Re6Se8I6]3â^' cluster. Its potential use as an antitumoral and biomarker agent. New Journal of Chemistry, 2012, 36, 927.	2.8	45
11	A TDâ€ĐFT basis set and density functional assessment for the calculation of electronic excitation energies of fluorene. International Journal of Quantum Chemistry, 2012, 112, 3434-3438.	2.0	44
12	Study of the structureâ€"bioactivity relationship of three new pyridine Schiff bases: synthesis, spectral characterization, DFT calculations and biological assays. New Journal of Chemistry, 2018, 42, 8851-8863.	2.8	41
13	Tellurium(0) as a Ligand: Synthesis and Characterization of 2-Pyridyltellurolates of Platinum(II) and Structures of [Pt{2-Te-3-(R)C₅H₃N}₂Te(PRâ€²₃)] (R = H or) Tj-ETQq1 1 0.78431	4.7	
14	Dirac scattered-wave calculations on an icosahedralAu13cluster. Physical Review B, 1987, 35, 3790-3798.	3.2	39
15	Oxidative Perhydroxylation of [closoâ€B₁₂H₁₂]^{2â^'} to the Stable Inorganic Cluster Redox System [B₁₂(OH)₁₂]^{2â^'/.â^'}: Experiment and Theory. Chemistry - A European Journal, 2010, 16, 11242-11245.	3.3	39
16	Calculated paramagnetic resonance parameters (g,A[sub hfi]) of the Re[sub 6]S[sub 8]Br[sub 6][sup 3â^'], Re[sub 6]S[sub 8]I[sub 6][sup 3â^'], and Re[sub 6]Se[sub 8]I[sub 6][sup 3â^'] cluster ions. Journal of Chemical Physics, 2003, 118, 7425.	3.0	38
17	Ground state of octahedral platinum hexafluoride. Physical Review A, 2008, 77, .	2.5	38
18	Luminescent europium(<scp>iii</scp>) and terbium(<scp>iii</scp>) complexes of Î²-diketonate and substituted terpyridine ligands: synthesis, crystal structures and elucidation of energy transfer pathways. New Journal of Chemistry, 2019, 43, 15139-15152.	2.8	38

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19	Spinâ€“orbit effects on the aromaticity of the Re3Cl9 and Re3Br9 clusters. Chemical Physics Letters, 2008, 467, 94-96.	2.6	37
20	Spinâ€“orbit effects on a gold-based superatom: a relativistic Jellium model. Physical Chemistry Chemical Physics, 2012, 14, 1408-1411.	2.8	36
21	Spin-orbit effects on electronic delocalization. Aromaticity in a discrete square tetrapalladium sandwich complex. Journal of Chemical Physics, 2010, 132, 164308.	3.0	34
22	Calculated optical and magnetic properties of hexafluorouranate (V) anion: UF[sub 6][sup â^']. Journal of Chemical Physics, 2004, 121, 7743.	3.0	32
23	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.	2.3	32
24	Electronic Delocalization, Energetics, and Optical Properties of Tripalladium Ditropylium Halides, [Pd₃(C₇H₇)₂X₃]^{1â^'} (X =) Tj ETQq0 0 0 rgBT /Overlock 1 5217-5221.	2.5	31
25	Calculated Molecular Properties of Triangular Tribenzo and Perfluoro-Tribenzo Trimercuronin Macrocycles. Journal of Physical Chemistry A, 2010, 114, 666-672.	2.5	29
26	Spinâ^'Orbit Effects on the Aromaticity of the Re₃X₉^{2â^'} (X = Cl, Br) Cluster Ions. Journal of Physical Chemistry A, 2009, 113, 1671-1673.	2.5	28
27	Understanding the Influence of Terminal Ligands on the Electronic Structure and Bonding Nature in [Re₆(Î¼₃-Q₈)]²⁺ Clusters. Journal of Physical Chemistry A, 2014, 118, 11083-11089.	2.5	28
28	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.	2.6	28
29	The luminescent [Mo6X8(NCS)6]2â^' (X=Cl, Br, I) clusters?: A computational study based on time-dependent density functional theory including spinâ€“orbit and solvent-polarity effects. Chemical Physics Letters, 2008, 455, 38-41.	2.6	27
30	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.	2.8	27
31	Nanostructuring of anodic copper oxides in fluoride-containing ethylene glycol media. Journal of Electroanalytical Chemistry, 2017, 807, 181-186.	3.8	27
32	Theoretical Determination of Energy Transfer Processes and Influence of Symmetry in Lanthanide(III) Complexes: Methodological Considerations. Inorganic Chemistry, 2018, 57, 5120-5132.	4.0	27
33	Calculated paramagnetic resonance parameters of the luminescent Re6S8Cl63â^' cluster ion. Journal of Chemical Physics, 2001, 115, 726-730.	3.0	25
34	Theoretical insights into the adsorption of neutral, radical and anionic thiophenols on gold(111). Physical Chemistry Chemical Physics, 2013, 15, 20363.	2.8	25
35	The Synthesis of Stable, Complex Organocesium Tetramic Acids through the Ugi Reaction and Cesiumâ€Carbonateâ€Promoted Cascades. Angewandte Chemie - International Edition, 2015, 54, 11672-11676.	13.8	25
36	Electronic Structure and Properties of Berkelium Iodates. Journal of the American Chemical Society, 2017, 139, 13361-13375.	13.7	25

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37	Rareâ€Earth Metal(II) Aryloxides: Structure, Synthesis, and EPR Spectroscopy of [K(2.2.2â€cryptand)][Sc(OC₆H₂tBu₂â€2,6â€Meâ€4)₃]. Chemistry - A European Journal, 2018, 24, 18059-18067.	3.3	25
38	Inside a Superatom: The M₇^q (M=Cu, Ag, q=1+, 0, 1â^') Case. ChemPhysChem, 2010, 11, 646-650.	2.1	24
39	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, .	1.2	24
40	Rhenium (I) Complexes as Probes for Prokaryotic and Fungal Cells by Fluorescence Microscopy: Do Ligands Matter?. Frontiers in Chemistry, 2019, 7, 454.	3.6	24
41	Two New Fluorinated Phenol Derivatives Pyridine Schiff Bases: Synthesis, Spectral, Theoretical Characterization, Inclusion in Epichlorohydrin-Î²-Cyclodextrin Polymer, and Antifungal Effect. Frontiers in Chemistry, 2018, 6, 312.	3.6	23
42	Cluster carbonyls of the [Re6(Î¼3-Se)8]2+ core: synthesis, structural characterization, and computational analysis. Dalton Transactions, 2008, , 4247.	3.3	22
43	Electronic structure, molecular properties and electronic currents of the luminescent [Au3(CH3NCOCH3)3] cluster. Chemical Physics Letters, 2009, 474, 290-293.	2.6	22
44	Bonding Nature and Electron Delocalization of An(COT)2, An = Th, Pa, U. Journal of Physical Chemistry A, 2011, 115, 8997-9003.	2.5	22
45	Coinage Metal Superatomic Cores: Insights into Their Intrinsic Stability and Optical Properties from Relativistic DFT Calculations. Chemistry - A European Journal, 2017, 23, 11330-11337.	3.3	22
46	Pyridine as axial ligand on the [Mo6Cl8]4+ core switches off luminescence. Chemical Physics Letters, 2009, 475, 232-234.	2.6	21
47	[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.	2.2	21
48	Theoretical and Experimental Study of Bonding and Optical Properties of Self-Assembly Metallophthalocyanines Complexes on a Gold Surface. A Survey of the Substrateâ€“Surface Interaction.. Journal of Physical Chemistry C, 2011, 115, 23512-23518.	3.1	21
49	Bonding in the octahedral Au62+ cluster. Chemical Physics Letters, 1986, 125, 143-148.	2.6	20
50	Calculated paramagnetic hyperfine structure of pentagonal bipyramid Ag7 cluster. Journal of Chemical Physics, 1998, 108, 5795-5798.	3.0	20
51	Direct Spectroscopic Evidence for Constituent Heteroatoms Enhancing Charge Recombination at a TiO₂â^'Ruthenium Dye Interface. Journal of Physical Chemistry C, 2014, 118, 17079-17089.	3.1	20
52	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.	2.6	20
53	Relativistic electronic structure of an icosahedral Au12Pd cluster. Chemical Physics Letters, 1999, 303, 641-648.	2.6	19
54	Relativistic molecular orbital study of the optical and magnetic properties of hexachloro protactinate (IV): PaCl62â^'. Journal of Chemical Physics, 2006, 124, 074321.	3.0	19

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55	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.	1.8	19
56	A Relativistic Study of the Electronic and Magnetic Properties of Cerocene and Thorocene and Its Anions. Journal of Physical Chemistry A, 2012, 116, 4170-4175.	2.5	19
57	Experimental and theoretical studies of the ancillary ligand (E)-2-((3-amino-pyridin-4-ylimino)-methyl)-4,6-di-tert-butylphenol in the rhenium(<scp>i</scp>) core. New Journal of Chemistry, 2015, 39, 5725-5734.	2.8	19
58	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.	2.8	19
59	Spinâ€"orbit effects on heavy metal octahedral clusters. Computational and Theoretical Chemistry, 1993, 282, 131-141.	1.5	18
60	Quantum relativistic investigation about the coordination and bonding effects of different ligands on uranyl complexes. Polyhedron, 2010, 29, 975-984.	2.2	18
61	Geometrically Specific Imino Complexes of the [Re₆(Î¼₃â€Se)₈]²⁺ Coreâ€Containing Clusters. Chemistry - A European Journal, 2011, 17, 580-587.	3.3	18
62	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.	2.6	18
63	Substituted bidentate and ancillary ligands modulate the bioimaging properties of the classical Re(<scp>i</scp>) tricarbonyl core with yeasts and bacteria. New Journal of Chemistry, 2017, 41, 2140-2147.	2.8	18
64	A DFT/TDDFT study of porphyrazines and phthalocyanine oxoâ€titanium derivatives as potential dyes in solar cells. International Journal of Quantum Chemistry, 2011, 111, 4186-4196.	2.0	17
65	New Insights into Re₃(Î¼-Cl)₃Cl₆ Aromaticity. Evidence of Ïƒ- and Ï€-Diatropicity. Journal of Physical Chemistry Letters, 2015, 6, 4326-4330.	4.6	17
66	Simulation of natural dyes adsorbed on TiO2 for photovoltaic applications. Solar Energy, 2017, 142, 215-223.	6.1	17
67	Reduction of Au(III) by a Î²-cyclodextrin polymer in acid medium. A stated unattainable reaction. Carbohydrate Polymers, 2017, 175, 530-537.	10.2	17
68	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.	3.0	17
69	The M6S8L6 clusters: an example in cluster and condensed phase chemistry. Chemical Physics Letters, 1993, 213, 547-553.	2.6	16
70	Cluster-Bound Nitriles Do Not Click with Organic Azides: Unexpected Formation of Imino Complexes of the [Re₆(Î¼₃-Se)₈]²⁺ Core-Containing Clusters. Inorganic Chemistry, 2010, 49, 380-382.	4.0	16
71	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.	2.6	16
72	Ï€-Donor/Acceptor Effect on Lindqvist Type Polyoxomolibdates Because of Various Multiple-Bonded Nitrogenous Ligands. Journal of Physical Chemistry A, 2007, 111, 6563-6567.	2.5	15

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73	Optical and Magnetic Properties of the Complex Bis(dicyclooctatetraenyl)diuranium. A Theoretical View. Organometallics, 2012, 31, 6297-6304.	2.3	15
74	The role of the [CpM(CO)₂]^{â^'} chromophore in the optical properties of the [Cp₂ThMCp(CO)₂]⁺ complexes, where M = Fe, Ru and Os. A theoretical view. Dalton Transactions, 2015, 44, 20004-20010.	3.3	15
75	Interaction of LD14 and TiO2 in dye-sensitized solar-cells (DSSC): A density functional theory study. Computational and Theoretical Chemistry, 2015, 1070, 117-125.	2.5	15
76	A Dirac molecular orbital study for hexanuclear tungsten cluster structures. Chemical Physics Letters, 1997, 277, 223-226.	2.6	14
77	Calculated paramagnetic resonance parameters of a gallium arsenide cluster: Ga2As3. Journal of Chemical Physics, 1998, 109, 3497-3500.	3.0	14
78	Relativistic scalar and spinâ€“orbit density functional calculations of the electronic structure, NICS index and ELF function of the [Re2(CO)8(Î¼-BiPh)2] and [Re2(CO)8(Î¼-BiPh2)2] clusters. Polyhedron, 2011, 30, 846-850.	2.2	14
79	Probing the aromaticity of the [(HtAc)3(Î¼2-H)6], [(HtTh)3(Î¼2-H)6],+, and [(HtPa)3(Î¼2-H)6] clusters. Journal of Chemical Physics, 2011, 135, 104506.	3.0	14
80	A new heterobimetallic manganeseâ€“rhodium carbonyl complex derived from partially alkylated s-indacene. Inorganica Chimica Acta, 2013, 394, 132-139.	2.4	14
81	Molecular and Electronic Structure, and Hydrolytic Reactivity of a Samarium(II) Crown Ether Complex. Inorganic Chemistry, 2019, 58, 3457-3465.	4.0	14
82	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.	1.5	13
83	Interaction of YD2 and TiO2 in dye-sensitized solar cells (DSSCs): a density functional theory study. Journal of Molecular Modeling, 2015, 21, 226.	1.8	13
84	Optical and electronic properties of benzopyrylium derivatives. Theoretical-experimental synergy towards novel DSSCs devices. Dyes and Pigments, 2019, 161, 370-381.	3.7	13
85	Electronic structure of tungsten hexacarbonyl. Chemical Physics Letters, 1984, 107, 112-116.	2.6	12
86	Photophysical properties of [Cu(binap)2]+ and [Pd(binap)2] complexes: A theoretical study. Polyhedron, 2012, 37, 54-59.	2.2	12
87	Role of the main adsorption modes in the interaction of the dye [COOHâ€“TPP-Zn(ii)] on a periodic TiO2 slab exposing a rutile (110) surface in a dye-sentized solar cell. RSC Advances, 2014, 4, 9639.	3.6	12
88	Surface on Surface. Survey of the Monolayer Goldâ€“Graphene Interaction from Au₁₂ and PAH via Relativistic DFT Calculations. Journal of Physical Chemistry C, 2016, 120, 7358-7364.	3.1	12
89	The origin of phosphorescence in Iridium (III) complexes. The role of relativistic effects. Chemical Physics Letters, 2017, 685, 60-68.	2.6	12
90	Electrochemical behaviors and relativistic DFT calculations to understand the terminal ligand influence on the [Re₆(Î¼₃-Q)₈X₆]^{4â^'} clusters. New Journal of Chemistry, 2018, 42, 5471-5478.	2.8	12

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91	Electronic structure of octachloroditungstate(II). Inorganic Chemistry, 1984, 23, 3271-3273.	4.0	11
92	Substituents Effects on Two Related Families of Dyes for Dye Sensitized Solar Cells: [Ru(4,4â€²-R,R-2,2â€²-bpy)₃]²⁺ and [Ru(4,4â€²-COOH-2,2â€²-bpy)(4,4â€²-R,R-2,2â€²-bpy)₂]²⁺. Journal of Physical Chemistry A, 2012, 116, 7436-7442.	2.5	11
93	Covalent lanthanide(<scp>iii</scp>) macrocyclic complexes: the bonding nature and optical properties of a promising single antenna molecule. Physical Chemistry Chemical Physics, 2014, 16, 25978-25988.	2.8	11
94	New bis(azolylcarbonyl)pyridine chromium(III) complexes as initiators for ethylene polymerization. Inorganica Chimica Acta, 2011, 378, 218-223.	2.4	10
95	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, 9931-9940.	2.5	10
96	Catalytic aspects of metallophthalocyanines adsorbed on gold-electrode. Theoretical exploration of the binding nature role. Physical Chemistry Chemical Physics, 2016, 18, 29516-29525.	2.8	10
97	Spinâ€”orbit effects on RuO4 and OsO4. Chemical Physics Letters, 1993, 203, 409-414.	2.6	9
98	Calculated paramagnetic properties of matrix isolated Au3 cluster. Chemical Physics Letters, 1995, 236, 37-42.	2.6	9
99	Calculated geometry and paramagnetic hyperfine structure of the Cu7 cluster. Chemical Physics Letters, 2004, 397, 408-411.	2.6	9
100	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, 1072-1077.	2.5	9
101	Toward the Synthetic Control of the HOMOâ^'LUMO Gap in Binuclear Systems: Insights from Density Functional Calculations. Inorganic Chemistry, 2010, 49, 4175-4178.	4.0	9
102	Antenna Effect by Organometallic Chromophores in Bimetallic dâ€“f Complexes. Journal of Physical Chemistry A, 2013, 117, 7847-7854.	2.5	9
103	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.	2.2	9
104	Relativistic effects in bonding and isomerization energy of the superheavy roentgenium (111Rg) cyanide. Polyhedron, 2012, 39, 113-117.	2.2	8
105	Effects of the peripheral substituents (â€“NH2, â€“OH, â€“CH3, â€“H, â€“C6H5, â€“Cl, â€“CO2H and â€“NO2) on molecular properties of a Ni-Porphyrazine dimers family. Polyhedron, 2013, 50, 131-138.	2.2	8
106	Exploring the nature of the excitation energies in [Re6(Î¼3-Q8)X6]4â^' clusters: a relativistic approach. Physical Chemistry Chemical Physics, 2015, 17, 17611-17617.	2.8	8
107	Theoretical exploration of seleno and tellurophenols as promising alternatives to sulfur ligands for anchoring to gold (111) materials. RSC Advances, 2016, 6, 4458-4468.	3.6	8
108	Three new types of transition metal carboranylamidinate complexes. Dalton Transactions, 2018, 47, 6666-6671.	3.3	8

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109	Calculated paramagnetic properties of the acute GaAs2 and obtuse Ga2As clusters. Journal of Chemical Physics, 1999, 110, 10882-10887.	3.0	7
110	Heterobimetallic Reî€Pd complexes bridged by Î·1:Î·5-Ph2PC5H4 ligand. Synthesis, electronic and crystal structure of (CO)2(PR3)(Î·5-C5H4î€PPh2)Reâ€“Pî€dCl2, R = Me and OMe. Dalton Transactions, 2010, 39, 6295.	3.3	7
111	Spinâ€“orbit effects on the optical and magnetic properties of cerium (III) hexahalides. Polyhedron, 2011, 30, 860-863.	2.2	7
112	Relativistic calculations of aminotroponiminate complexes containing group 15 (P, As, Sb, Bi) elements. Polyhedron, 2011, 30, 841-845.	2.2	7
113	Bonding, energetic, electronic delocalization and optical properties of MCp3 complexes, where M=Sc, Y, La, Ac, Lu, Ce, Yb and Th. Chemical Physics Letters, 2012, 554, 219-224.	2.6	7
114	The aromaticity of the [Re3(Î¼-X)3X9]3â^' clusters, X=Cl, Br, I. Chemical Physics Letters, 2012, 545, 50-53.	2.6	7
115	Density functional study on Keggin heteropolyanions containing fifth period main group heteroatoms. Polyhedron, 2016, 117, 478-486.	2.2	7
116	Spin-orbit effect into isomerization barrier of small gold Clusters. Ohâ†”D2h Fluxionality of the Au62+ cluster Investigated by relativistic methods. Chemical Physics Letters, 2017, 683, 404-407.	2.6	7
117	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.	2.2	7
118	Synthesis, characterization and relativistic DFT studies of fac -Re(CO) 3 (isonicotinic acid) 2 Cl complex. Chemical Physics Letters, 2017, 688, 66-73.	2.6	7
119	[M₁₆Ni₂₄(CO)₄₀]^{4â€“}: 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.	3.1	7
120	The role of zero-field splitting and Ï€-stacking interaction of different nitrogen-donor ligands on the optical properties of luminescent rhenium tricarbonyl complexes. New Journal of Chemistry, 2021, 45, 11192-11201.	2.8	7
121	Paramagnetic resonance hyperfine structure of hexachloroprotactinate(IV). Physical Review B, 1988, 37, 4893-4899.	3.2	6
122	Calculated Paramagnetic Hyperfine Structure of the C2v Isomers of Ag3. The Journal of Physical Chemistry, 1994, 98, 5627-5631.	2.9	6
123	A Dirac molecular orbital study for the tetragonal compression in the RuY6I122â^' cluster. Chemical Physics Letters, 1996, 255, 217-222.	2.6	6
124	Electronic structure and metalâ€“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.	2.8	6
125	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.	1.2	6
126	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.	2.6	6

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127	Electronic structure and molecular properties of paramagnetic hexanuclear Tantalum [Ta6X12Y6]3â^' (X) Tj ETQq1 1 0.784314 rgBT /	2.2	6
128	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.	1.8	6
129	Bonding in gold-rare earth [Au2M] (M = Eu, Yb, Lu) ions. A strong covalent gold-lanthanide bond. Chemical Physics Letters, 2017, 683, 421-424.	2.6	6
130	X-ray diffraction and relativistic DFT studies on the molecular biomarker fac-Re(CO)3(4,4â€²-dimethyl-2,2â€²-bpy)(E-2-((3-amino-pyridin-4-ylimino)-methyl)-4,6-di-tert-butylphenol)(PF6). Chemical Papers, 2017, 71, 2011-2022.	2.2	6
131	Aromaticity of [M₃(Âµâ€X)₃X₆]^{0/2â€“} (M = Re and Tc, X =) Tj ETQq1 1 0.78431 Inorganic Chemistry, 2018, 2018, 3312-3319.	2.0	6
132	Insights into the role of Dâ€Aâ€Ïâ€A type proâ€aromatic organic dyes with thieno[3,4â€b]pyrazine as A acceptor group into dyeâ€sensitized solarâ€cells. A TDâ€DFT/periodic DFT study. International Journal of Quantum Chemistry, 2020, 120, e26108.	2.0	6
133	Geometry, bonding and optical and magnetic properties of copper tricarbonyl: a theoretical study. The Journal of Physical Chemistry, 1987, 91, 5177-5183.	2.9	5
134	Relativistic electronic structure of staggered and eclipsed conformations of octachlorodiosmate(III). The Journal of Physical Chemistry, 1991, 95, 7239-7244.	2.9	5
135	A Dirac molecular orbital study for encapsulated heavy transition metals within ytrium cluster iodides. Chemical Physics Letters, 1995, 247, 163-167.	2.6	5
136	Electronic structure and molecular properties of the octacyanorhenate [Re(CN)8]3â^' and [Re(CN)8]2â^' complexes. Chemical Physics Letters, 2006, 422, 89-94.	2.6	5
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