Ramiro Arratia-Perez

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Revising the formation and electronic properties in flavylium derivatives. A theoretical tandem towards optimized DSSCs. *New Journal of Chemistry*, **2021**, 45, 4453-4463	3.6	0
165	The role of zero-field splitting and □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
164	Role of donor-acceptor functional groups in N3P3 cyclic-triphosphazene backbone. Unraveling bonding characteristics from natural orbitals within an extended transition state-natural orbital for the chemical valence scheme. *International Journal of Quantum Chemistry*, **2020**, 120, e26057	2.1	
163	Insights into the role of D-A-□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
162	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
161	Catalytic activity of a new Ru(II) complex for the hydrogen transfer reaction of acetophenone and N-benzylideneaniline: synthesis, characterization and relativistic DFT approaches. *New Journal of Chemistry*, **2019**, 43, 10545-10553	3.6	1
160	Rhenium Hexanuclear Clusters: Bonding, Spectroscopy, and Applications of Molecular Chevrel Phases. *Structure and Bonding*, **2019**, 109-123	0.9	1
159	Potential to stabilize 16-vertex tetrahedral coinage-metal cluster architectures related to Au. *Physical Chemistry Chemical Physics*, **2019**, 21, 8428-8433	3.6	3
158	Classical and Quantum Mechanical Calculations of the Stacking Interaction of Nd Complexes with Regular and Mismatched DNA Sequences. *Journal of Physical Chemistry B*, **2019**, 123, 3219-3231	3.4	3
157	Stabilizing heteroatom-centered 16-vertex group 11 tetrahedral architectures: Bonding and structural considerations toward versatile endohedral species. *International Journal of Quantum Chemistry*, **2019**, 119, e26038	2.1	
156	Rhenium (I) Complexes as Probes for Prokaryotic and Fungal Cells by Fluorescence Microscopy: Do Ligands Matter?. *Frontiers in Chemistry*, **2019**, 7, 454	5	15
155	Molecular and Electronic Structure, and Hydrolytic Reactivity of a Samarium(II) Crown Ether Complex. *Inorganic Chemistry*, **2019**, 58, 3457-3465	5.1	8
154	Optical and electronic properties of benzopyrylium derivatives. Theoretical-experimental synergy towards novel DSSCs devices. *Dyes and Pigments*, **2019**, 161, 370-381	4.6	12
153	Symmetry lowering by cage doping in spherical superatoms: Evaluation of electronic and optical properties of 18-electron W@Au12Pt n (n = 0-4) superatomic clusters from relativistic DFT calculations. *International Journal of Quantum Chemistry*, **2019**, 119, e25827	2.1	
152	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
151	Advances in bonding and properties of inorganic systems from relativistic calculations in Latin America. *International Journal of Quantum Chemistry*, **2019**, 119, e25777	2.1	3
150	Electrochemical behaviors and relativistic DFT calculations to understand the terminal ligand influence on the [Re6(□-Q)8X6]4□clusters. *New Journal of Chemistry*, **2018**, 42, 5471-5478	3.6	11

149	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
148	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
147	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
146	Three new types of transition metal carboranylamidinate complexes. *Dalton Transactions*, **2018**, 47, 6666-6671	4	4
145	Comparative study of the anchorage and the catalytic properties of nanoporous TiO2 films modified with ruthenium (II) and rhenium (I) carbonyl complexes. *Chemical Physics Letters*, **2018**, 694, 40-47	2.5	4
144	[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
143	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
142	A theoretical study of the super exchange mechanism and magneto-structural relationships in the [Mn(III)2(μ-F)F4(Me3tacn)2](PF6) coordination compound. *New Journal of Chemistry*, **2018**, 42, 13847-13855	3.6	1
141	Magnetically induced current density using London atomic orbitals of dihydroindeno-[1,2-b]-fluorenes. *New Journal of Chemistry*, **2018**, 42, 15648-15654	3.6	1
140	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
139	Simple and Rapid One-Step Electrochemical Synthesis of Nanogranular Cu2O Films. *ChemistrySelect* , **2018**, 3, 8610-8614	1.8	2
138	Aromaticity of [M3(μ-X)3X6]0/2− (M = Re and Tc, X = Cl, Br, I) Clusters Confirmed by Ring Current Analysis and Induced Magnetic Field. *European Journal of Inorganic Chemistry*, **2018**, 2018, 3312-3319	2.3	4
137	In-Situ Preparation of CdTe Quantum Dots Capped with a β-Cyclodextrin-Epichlorohydrin Polymer: Polymer Influence on the Nanocrystal's Optical Properties. *Nanomaterials*, **2018**, 8,	5.4	2
136	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
135	Tuning the molecular antenna effect using donor and acceptor substituents on the optical properties of the [(C5F5)2ThMCp2]2+ and [(C5F5)2ThMCpL2]+ complexes, where M = Fe, Ru and Os and L = CO and C5H5N. *New Journal of Chemistry*, **2018**, 42, 11013-11022	3.6	4
134	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
133	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
132	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

131	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
130	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
129	Simulation of natural dyes adsorbed on TiO2 for photovoltaic applications. *Solar Energy*, **2017**, 142, 215-223	3.3	17
128	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
127	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
126	Reduction of Au(III) by a Ecyclodextrin polymer in acid medium. A stated unattainable reaction. *Carbohydrate Polymers*, **2017**, 175, 530-537	10.3	14
125	Electronic Structure and Properties of Berkelium Iodates. *Journal of the American Chemical Society*, **2017**, 139, 13361-13375	16.4	18
124	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
123	Nanostructuring of anodic copper oxides in fluoride-containing ethylene glycol media. *Journal of Electroanalytical Chemistry*, **2017**, 807, 181-186	4.1	19
122	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
121	The origin of phosphorescence in Iridium (III) complexes. The role of relativistic effects. *Chemical Physics Letters*, **2017**, 685, 60-68	2.5	8
120	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
119	Surface on Surface. Survey of the Monolayer GoldGraphene Interaction from Au12 and PAH via Relativistic DFT Calculations. *Journal of Physical Chemistry C*, **2016**, 120, 7358-7364	3.8	8
118	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
117	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
116	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
115	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
114	Density functional study on Keggin heteropolyanions containing fifth period main group heteroatoms. *Polyhedron*, **2016**, 117, 478-486	2.7	6

113	Insights into bonding interactions and excitation energies of 3d-4f mixed lanthanide transition metal macrocyclic complexes. *Physical Chemistry Chemical Physics*, **2016**, 18, 33218-33225	3.6	3
112	Theoretical Aspects of the Reactivity of MN4 Macrocyclics in Electrochemical Reactions **2016**, 143-170		1
111	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
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	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
108	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
107	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
106	New Insights into Re3(□Cl)3Cl6 Aromaticity. Evidence of □and □Diatropicity. *Journal of Physical Chemistry Letters*, **2015**, 6, 4326-30	6.4	14
105	Interaction of YD2 and TiO□n dye-sensitized solar cells (DSSCs): a density functional theory study. *Journal of Molecular Modeling*, **2015**, 21, 226	2	12
104	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
103	Computational study of organo-cesium complexes and the possibility of lanthanide/actinide ions substitution. *Chemical Physics Letters*, **2015**, 641, 181-186	2.5	
102	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
101	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
100	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
99	Exploring the nature of the excitation energies in [Re6(□-Q8)X6](4-) clusters: a relativistic approach. *Physical Chemistry Chemical Physics*, **2015**, 17, 17611-7	3.6	8
98	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
97	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
96	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

95	Understanding the influence of terminal ligands on the electronic structure and bonding nature in [Re6(□3-Q8)](2+) clusters. *Journal of Physical Chemistry A*, **2014**, 118, 11083-9	2.8	15
94	Intramolecular and lateral intermolecular hole transfer at the sensitized TiO2 interface. *Journal of the American Chemical Society*, **2014**, 136, 1034-46	16.4	51
93	Role of the main adsorption modes in the interaction of the dye [COOH□PP-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
92	Antenna effect by organometallic chromophores in bimetallic d-f complexes. *Journal of Physical Chemistry A*, **2013**, 117, 7847-54	2.8	8
91	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
90	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
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	Novel titanocene derived from a partially alkylated s-indacene: Synthesis, characterization and comparative study with its zirconium analog. *Inorganica Chimica Acta*, **2013**, 396, 35-39	2.7	2
87	Effects of the peripheral substituents (□NH2, □OH, □CH3, □H, □C6H5, □Cl, □CO2H and □NO2) on molecular properties of a Ni-Porphyrazine dimers family. *Polyhedron*, **2013**, 50, 131-138	2.7	4
86	THEORETICAL CALCULATIONS OF AN OSMIUM MOLECULAR SWITCH. *Journal of the Chilean Chemical Society*, **2013**, 58, 2110-2113	2.5	1
85	RELATIVISTIC-DFT STUDY OF THE ELECTRONIC STRUCTURE, BONDING AND ENERGETIC OF THE [ReF8]־ AND [UF8]2- IONS. *Journal of the Chilean Chemical Society*, **2013**, 58, 2020-2024	2.5	1
84	Theoretical study of 3,3? substitution of 9,9,9?,9?-tetramethyl-fluorene-dimers. *Chemical Physics Letters*, **2012**, 538, 67-71	2.5	1
83	Charge transfer effects on the paramagnetic properties of the [M(C8H8)2] and M(C5H5)(C8H8); M = Ti, Zr, Hf and Th, complexes. *Polyhedron*, **2012**, 36, 69-72	2.7	3
82	Photophysical properties of [Cu(binap)2]+ and [Pd(binap)2] complexes: A theoretical study. *Polyhedron*, **2012**, 37, 54-59	2.7	9
81	Electronic structure and molecular properties of paramagnetic hexanuclear Tantalum [Ta6X12Y6]3□(X and Y=F, Cl, Br, I) cluster compounds. *Polyhedron*, **2012**, 36, 127-132	2.7	4
80	Relativistic effects in bonding and isomerization energy of the superheavy roentgenium (111Rg) cyanide. *Polyhedron*, **2012**, 39, 113-117	2.7	8
79	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
78	Spin-orbit effects on a gold-based superatom: a relativistic Jellium model. *Physical Chemistry Chemical Physics*, **2012**, 14, 1408-11	3.6	33

77	Optical and Magnetic Properties of the Complex Bis(dicyclooctatetraenyl)diuranium. A Theoretical View. *Organometallics*, **2012**, 31, 6297-6304	3.8	15
76	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
75	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	2.5	4
74	The aromaticity of the [Re3(□X)3X9]3□clusters, X = Cl, Br, I. *Chemical Physics Letters*, **2012**, 545, 50-53	2.5	6
73	Aromaticity, optical properties and zero field splitting of homo- and hetero-bimetallic (C8H8)M(□-,□?C8H8)M(C8H8) where M = Ti, Zr, Th Complexes. *Journal of Physical Chemistry A*, **2012**, 116, 7584-92	2.8	2
72	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
71	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
70	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
69	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
68	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
67	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
66	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
65	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
64	New bis(azolylcarbonyl)pyridine chromium(III) complexes as initiators for ethylene polymerization. *Inorganica Chimica Acta*, **2011**, 378, 218-223	2.7	9
63	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
62	Geometrically specific imino complexes of the [Re6(□-Se)8]2+ core-containing clusters. *Chemistry - A European Journal*, **2011**, 17, 580-7	4.8	18
61	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
60	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

59	Spin□orbit effects on the optical and magnetic properties of cerium (III) hexahalides. *Polyhedron*, **2011**, 30, 860-863	2.7	7
58	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
57	Relativistic calculations of aminotroponiminate complexes containing group 15 (P, As, Sb, Bi) elements. *Polyhedron*, **2011**, 30, 841-845	2.7	6
56	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
55	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
54	Spin-orbit effects on electronic delocalization. Aromaticity in a discrete square tetrapalladium sandwich complex. *Journal of Chemical Physics*, **2010**, 132, 164308	3.9	33
53	Calculated molecular properties of triangular tribenzo and perfluoro-tribenzo trimercuronin macrocycles. *Journal of Physical Chemistry A*, **2010**, 114, 666-72	2.8	26
52	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
51	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
50	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
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	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
47	Inside a superatom: the M7q (M=Cu, Ag, q=1+, 0, 1-) case. *ChemPhysChem*, **2010**, 11, 646-50	3.2	23
46	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
45	Quantum relativistic investigation about the coordination and bonding effects of different ligands on uranyl complexes. *Polyhedron*, **2010**, 29, 975-984	2.7	17
44	[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
43	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
42	DFT-modeling of the tungsten (V) cofactor of hyperthermophilic Pyrococcus furiosus tungsto-bispterin enzyme via the calculated EPR parameters. *Chemical Physics Letters*, **2010**, 491, 214-217	2.5	1

41	Reply to Comment on Ground state of octahedral platinum hexafluoride. *Physical Review A*, **2009**, 79,	2.6	2
40	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
39	Electronic structure, molecular properties and electronic currents of the luminescent [Au3(CH3NCOCH3)3] cluster. *Chemical Physics Letters*, **2009**, 474, 290-293	2.5	22
38	Pyridine as axial ligand on the [Mo6Cl8]4+ core switches off luminescence. *Chemical Physics Letters*, **2009**, 475, 232-234	2.5	20
37	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
36	Ground state of octahedral platinum hexafluoride. *Physical Review A*, **2008**, 77,	2.6	33
35	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
34	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
33	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
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