Santiago Alvarez

List of Publications by Citations

291 papers	20,007 citations	67 h-index	135 g-index
309 ext. papers	21,474 ext. citations	6.7 avg, IF	6.98 L-index

#	Paper	IF	Citations
291	Covalent radii revisited. *Dalton Transactions*, **2008**, 2832-8	4.3	2540
290	A cartography of the van der Waals territories. *Dalton Transactions*, **2013**, 42, 8617-36	4.3	838
289	Broken symmetry approach to calculation of exchange coupling constants for homobinuclear and heterobinuclear transition metal complexes **1999**, 20, 1391-1400		779
288	Toward the Prediction of Magnetic Coupling in Molecular Systems: Hydroxo- and Alkoxo-Bridged Cu(II) Binuclear Complexes. *Journal of the American Chemical Society*, **1997**, 119, 1297-1303	16.4	773
287	Shape maps and polyhedral interconversion paths in transition metal chemistry. *Coordination Chemistry Reviews*, **2005**, 249, 1693-1708	23.2	727
286	Magnetic Coupling in End-On Azido-Bridged Transition Metal Complexes: A Density Functional Study. *Journal of the American Chemical Society*, **1998**, 120, 11122-11129	16.4	633
285	The rich stereochemistry of eight-vertex polyhedra: a continuous shape measures study. *Chemistry - A European Journal*, **2005**, 11, 1479-94	4.8	540
284	About the calculation of exchange coupling constants in polynuclear transition metal complexes. *Journal of Computational Chemistry*, **2003**, 24, 982-9	3.5	442
283	Structural Modeling and Magneto-Structural Correlations for Hydroxo-Bridged Copper(II) Binuclear Complexes. *Inorganic Chemistry*, **1997**, 36, 3683-3688	5.1	364
282	Continuous symmetry maps and shape classification. The case of six-coordinated metal compounds. *New Journal of Chemistry*, **2002**, 26, 996-1009	3.6	330
281	Exchange coupling in carboxylato-bridged dinuclear copper(II) compounds: a density functional study. *Chemistry - A European Journal*, **2001**, 7, 627-37	4.8	315
280	About the calculation of exchange coupling constants using density-functional theory: the role of the self-interaction error. *Journal of Chemical Physics*, **2005**, 123, 164110	3.9	299
279	Minimal distortion pathways in polyhedral rearrangements. *Journal of the American Chemical Society*, **2004**, 126, 1755-63	16.4	294
278	Distortions in Octahedrally Coordinated d0 Transition Metal Oxides: A Continuous Symmetry Measures Approach. *Chemistry of Materials*, **2006**, 18, 3176-3183	9.6	278
277	Polyhedral structures with an odd number of vertices: nine-coordinate metal compounds. *Chemistry - A European Journal*, **2008**, 14, 1291-303	4.8	245
276	Dimerization and stacking in transition-metal bisdithiolenes and tetrathiolates. *Journal of the American Chemical Society*, **1985**, 107, 6253-6277	16.4	213
275	Coordinating ability of anions and solvents towards transition metals and lanthanides. *Dalton Transactions*, **2011**, 40, 10742-50	4.3	206

274	Dihydrogen contacts in alkanes are subtle but not faint. *Nature Chemistry*, **2011**, 3, 323-30	17.6	199
273	Exchange coupling of transition-metal ions through hydrogen bonding: a theoretical investigation. *Journal of the American Chemical Society*, **2002**, 124, 5197-205	16.4	190
272	Exchange Coupling in Oxalato-Bridged Copper(II) Binuclear Compounds: A Density Functional Study. *Chemistry - A European Journal*, **1998**, 4, 476-484	4.8	185
271	Can large magnetic anisotropy and high spin really coexist?. *Chemical Communications*, **2008**, 52-4	5.8	184
270	Choice of coordination number in d10 complexes of group 11 metals. *Journal of the American Chemical Society*, **2004**, 126, 1465-77	16.4	184
269	Shape and symmetry of heptacoordinate transition-metal complexes: structural trends. *Chemistry - A European Journal*, **2003**, 9, 1281-95	4.8	183
268	Spin Density Distribution in Transition Metal Complexes: Some Thoughts and Hints. *Comments on Inorganic Chemistry*, **1998**, 20, 27-56	3.9	180
267	Binuclear and polymeric gold(I) complexes. *Inorganic Chemistry*, **1985**, 24, 749-757	5.1	161
266	Spin density distribution in transition metal complexes. *Coordination Chemistry Reviews*, **2005**, 249, 2649-2660	23.2	153
265	Mapping the stereochemistry and symmetry of tetracoordinate transition-metal complexes. *Chemistry - A European Journal*, **2004**, 10, 190-207	4.8	152
264	Influence of the Peripheral Ligand Atoms on the Exchange Interaction in Oxalato-Bridged Nickel(II) Complexes: An Orbital Model. Crystal Structures and Magnetic Properties of (H(3)dien)(2)[Ni(2)(ox)(5)].12H(2)O and [Ni(2)(dien)(2)(H(2)O)(2)(ox)]Cl(2). *Inorganic Chemistry*, **1996**, 35, 3741-3751	5.1	151
263	Spin state behavior of iron(II)/dipyrazolylpyridine complexes. New insights from crystallographic and solution measurements. *Coordination Chemistry Reviews*, **2015**, 289-290, 2-12	23.2	148
262	Theoretical study of exchange coupling in 3d-Gd complexes: large magnetocaloric effect systems. *Journal of the American Chemical Society*, **2012**, 134, 10532-42	16.4	144
261	Structural and electronic effects on the exchange interactions in dinuclear bis(phenoxo)-bridged copper(II) complexes. *Coordination Chemistry Reviews*, **2010**, 254, 2086-2095	23.2	142
260	Magnetic coupling in end-to-end azido-bridged copper and nickel binuclear complexes: a theoretical study. *Inorganic Chemistry*, **2000**, 39, 3221-9	5.1	140
259	How to build molecules with large magnetic anisotropy. *Chemistry - A European Journal*, **2009**, 15, 4078-87	4.8	139
258	Electronic structure and properties of Cu2O. *Physical Review B*, **1997**, 56, 7189-7196	3.3	131
257	Shape and spin state in four-coordinate transition-metal complexes: the case of the d(6) configuration. *Chemistry - A European Journal*, **2006**, 12, 3162-7	4.8	131

256	Oxalato-bridged and related dinuclear copper(II) complexes: theoretical analysis of their structures and magnetic coupling. *Inorganic Chemistry*, **1990**, 29, 4500-4507	5.1	131
255	The nature of intermolecular CuI...CuI interactions: a combined theoretical and structural database analysis. *Chemistry - A European Journal*, **2004**, 10, 2117-32	4.8	130
254	Is it possible to get high T(C) magnets with Prussian blue analogues? A theoretical prospect. *Chemistry - A European Journal*, **2005**, 11, 2135-44	4.8	123
253	Electronic structure and properties of AlN. *Physical Review B*, **1994**, 49, 7115-7123	3.3	123
252	To Bend or Not To Bend: Dilemma of the Edge-Sharing Binuclear Square Planar Complexes of d8 Transition Metal Ions. *Inorganic Chemistry*, **1998**, 37, 804-813	5.1	117
251	Continuous symmetry measures of penta-coordinate molecules: Berry and non-Berry distortions of the trigonal bipyramid. *Dalton Transactions RSC*, **2000**, 3288-3303		115
250	Distortion Pathways of Transition Metal Coordination Polyhedra Induced by Chelating Topology. *Chemical Reviews*, **2015**, 115, 13447-83	68.1	114
249	Exchange coupling in halo-bridged dinuclear Cu(II) compounds: a density functional study. *Inorganic Chemistry*, **2002**, 41, 3769-78	5.1	114
248	Polyhedra in (inorganic) chemistry. *Dalton Transactions*, **2005**, 2209-33	4.3	113
247	Importance of the X4 ring orbitals for the semiconducting, metallic, or superconducting properties of skutterudites MX3 and RM4X12. *Inorganic Chemistry*, **1990**, 29, 2252-2255	5.1	108
246	Density functional study of magnetostructural correlations in cubane complexes containing the Cu4O4 core. *Journal of Materials Chemistry*, **2006**, 16, 2729-2735		100
245	Continuous Shape Measures as a Stereochemical Tool in Organometallic Chemistry. *Organometallics*, **2005**, 24, 1556-1562	3.8	99
244	Ligand macrocycle structural effects on copper-dioxygen reactivity. *Inorganic Chemistry*, **2000**, 39, 4059-72	5.1	98
243	From Widely Accepted Concepts in Coordination Chemistry to Inverted Ligand Fields. *Chemical Reviews*, **2016**, 116, 8173-92	68.1	94
242	Stereochemistry of compounds with coordination number ten. *Chemistry - A European Journal*, **2009** , 15, 7470-80	4.8	92
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237	Magnetostructural correlations in polynuclear complexes: the Fe4 butterflies. *Journal of the American Chemical Society*, **2006**, 128, 15722-7	16.4	88
236	Density functional study of the exchange coupling in distorted cubane complexes containing the Cu4O4 core. *Polyhedron*, **2001**, 20, 1323-1327	2.7	87
235	On the Bonding Nature of the M.cntdot. .cntdot. .cntdot.M Interactions in Dimers of Square-Planar Pt(II) and Rh(I) Complexes. *Journal of the American Chemical Society*, **1995**, 117, 7169-7171	16.4	87
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204	Interconversion of quadruply and quintuply bonded molybdenum complexes by reductive elimination and oxidative addition of dihydrogen. *Angewandte Chemie - International Edition*, **2013**, 52, 3227-31	16.4	45
203	Reply to "Comment on 'About the calculation of exchange coupling constants using density-functional theory: The role of the self-interaction error' [J. Chem. Phys. 123, 164110 (2005)]". *Journal of Chemical Physics*, **2006**, 124, 107102	3.9	44

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178	Hexakis(silyl)palladium(VI) or Palladium(II) with □2-Disilane Ligands? This work was supported by the Direcci□ General de Ense□anza Superior (DGES), grant PB98-1166-C02-01, and the Comissionat per a Universitats i Recerca (Generalitat de Catalunya), grant SGR99-0046. Computing resources at the Centre de Supercomputaci□ de Catalunya (CESCA) and Centre de Paral?lelisme de Barcelona	16.4	31
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