F Aguilera-Granja

List of Publications by Year
in descending order

117	2,122	257450	289244
papers	citations	24 h-index	40 g-index

119	119	119	1485
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Hollow structures of Ti O systems with m â‰ˆ 2n: A density functional theoretical study. Journal of Physics and Chemistry of Solids, 2022, 164, 110646.	4.0	1
2	Relation between structural patterns and magnetism in small iron oxide clusters: reentrance of the magnetic moment at high oxidation ratios. Physical Chemistry Chemical Physics, 2021, 23, 246-272.	2.8	10
3	TiO2 nano-clusters adsorbed on surfaces: A density-functional-theoretic study. Journal of Physics and Chemistry of Solids, 2021, 150, 109716.	4.0	5
4	Bimetalic (AuPt)4 nano-clusters adsorbed on TiO2 nano-wires: A density-functional-theoretic study. Journal of Physics and Chemistry of Solids, 2021, 159, 110275.	4.0	3
5	Magnetism and Distortions in Two-Dimensional Transition-Metal Dioxides: On the Quest for Intrinsic Magnetic Semiconductor Layers. Journal of Physical Chemistry C, 2020, 124, 2634-2643.	3.1	11
6	Tuning the Magnetic Moment of Small Late 3d-Transition-Metal Oxide Clusters by Selectively Mixing the Transition-Metal Constituents. Nanomaterials, 2020, 10, 1814.	4.1	2
7	Structural, electronic and catalytic properties of bimetallic Pt Ag (n=1â€“7) clusters. Journal of Alloys and Compounds, 2020, 845, 155897.	5.5	15
8	Structural and electronic properties of (TiO2)10 clusters with impurities: A density functional theory investigation. Journal of Physics and Chemistry of Solids, 2019, 135, 109107.	4.0	6
9	A first principles systematic study of the structural, electronic, and magnetic properties of Heusler X₂MnZ with X = Fe, Co, Ni, Cu, Ru, Rh, Pd, Ag, Pt, Au and Z = Al, Si, Ga, Ge, In and Sn. Materials Research Express, 2019, 6, 106118.	1.6	17
10	Structure, fragmentation patterns, and electronic properties of small indium oxide clusters. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	2
11	Structural and electronic properties of (TiO 2) N nanowires: A density functional theory investigation. Journal of Physics and Chemistry of Solids, 2018, 119, 175-182.	4.0	4
12	Structure, fragmentation patterns, and magnetic properties of small nickel oxide clusters. Physical Chemistry Chemical Physics, 2017, 19, 3366-3383.	2.8	12
13	New structural and electronic properties of (TiO2)10. Journal of Chemical Physics, 2016, 144, 234312.	3.0	13
14	Structural, electronic, and magnetic properties of Fe x Co y Pd z (xÂ+ÂyÂ+ÂzÂâ‰Â7) clusters: a density functional theory study. Journal of Nanoparticle Research, 2016, 18, 1.	1.9	12
15	Structural, Vibrational, and Magnetic Properties of FeCoO_n^{0/+} (n = 1â€“6) Bimetallic Oxide Clusters. Journal of Physical Chemistry C, 2015, 119, 11200-11209.	3.1	5
16	Structural, electronic, and magnetic properties of Fe Co Ni (<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 157 Td (xmlns:mml="http clusters: A density-functional-theory study. Journal of Magnetism and Magnetic Materials, 2015, 394, 325-334.	2.3	30
17	Breakdown of magnetism in sub-nanometric Ni clusters embedded in Ag. Nanotechnology, 2015, 26, 455703.	2.6	11
18	Titanium embedded cage structure formation in AlnTi+ clusters and their interaction with Ar. Journal of Chemical Physics, 2014, 140, 174304.	3.0	1

#	Article	IF	Citations
19	Spinâ€“orbit effects on the structural, homotop, and magnetic configurations of small pure and Fe-doped Pt clusters. Journal of Nanoparticle Research, 2014, 16, 1.	1.9	8
20	Structural, electronic and magnetic properties of , for M=13, 19, and 55, from first principles. Journal of Magnetism and Magnetic Materials, 2014, 355, 215-224.	2.3	23
21	Structural and Electronic Properties of TM_n[(BN)₃H₆]_m Complexes with TM = Co (n, m = 1â€“3) and with TM = Fe, Ni, Ru, Rh, Pd (n = m = 1â€“3). Journal of Physical Chemistry A, 2014, 118, 2976-2983.	2.5	7
22	Structure, fragmentation patterns, and magnetic properties of small cobalt oxide clusters. Physical Chemistry Chemical Physics, 2014, 16, 21732-21741.	2.8	25
23	Antiferromagnetic-like coupling in the cationic iron cluster of thirteen atoms. Physical Chemistry Chemical Physics, 2013, 15, 14458.	2.8	15
24	A new family of star-like icosahedral structures for small cobalt clusters. Chemical Physics, 2013, 415, 106-111.	1.9	12
25	Structural and electronic properties of Ni26â€“p X p clusters (X = Pd, Pt): A density-functional-theoretic study. Journal of Applied Physics, 2013, 114, .	2.5	16
26	Hydrogen Interaction in Pdâ€“Pt Alloy Nanoparticles. Journal of Physical Chemistry C, 2012, 116, 126-133.	3.1	28
27	Hybrid density functional study of small Rh<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>n</mml:mi></mml:msub></mml:math><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mo>(</mml:mo><mml:mi>n</mml:mi><mml:mo>=</mml:mo><mml:mn>2</mml:mn><mml:mo>	3.2	36
28	Structural, Electronic, and Magnetic Properties Of Co_nCu_m Nanoalloys (m + n = 12) from First Principles Calculations. Journal of Physical Chemistry A, 2012, 116, 9353-9360.	2.5	14
29	Magnetic Cooperative Effects in Small Niâ€“Ru Clusters. Journal of Physical Chemistry A, 2011, 115, 13950-13955.	2.5	10
30	Stability, structural, and magnetic phase diagrams of ternary ferromagnetic 3d-transition-metal clusters with five and six atoms. Journal of Chemical Physics, 2011, 134, 054101.	3.0	29
31	Hydrogen insertion in Pd core/Pt shell cubo-octahedral nanoparticles. Physical Review B, 2011, 83, .	3.2	12
32	Ab Initio Study of the Adsorption of NO on the Rh6+Cluster. Journal of Physical Chemistry A, 2011, 115, 8350-8360.	2.5	25
33	Structural and magnetic properties of FemYn (mÂ+ÂnÂ=Â7, Y = Ru, Rh, Pd, and Pt) nanoalloys. European Physical Journal D, 2011, 64, 53-62.	1.3	16
34	DFT and GEGA genetic algorithm optimized structures of Cun Î½ (Î½=Â±1,0,2; n=3-13) clusters. European Physical Journal D, 2010, 57, 49-60.	1.3	50
35	Theoretical study of bimetallic magnetic nanostructures: ConPdN-n, n=0,1,...N, N=3,5,7,13. European Physical Journal D, 2010, 57, 61-69.	1.3	19
36	DFT study of the fragmentation channels and electronic properties of Cu n Î½ (Î½= Â±1,0,2; n=3-13) clusters. European Physical Journal D, 2010, 57, 335-342.	1.3	19

#	Article	IF	Citations
37	Structural and magnetic properties of X12Y (X, Y=Fe, Co, Ni, Ru, Rh, Pd, and Pt) nanoalloys. Journal of Chemical Physics, 2010, 132, .	3.0	61
38	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Mo</mml:mtext></mml:mrow><mml:mrow><mml:mn>4</mml:m Structural transition and electronic structure of interest in spintronics. Physical Review B, 2009, 79, .	3.2	14
39	Study of the Structural and Electronic Properties of Rh_N and Ru_N Clusters (N < 20) within the Density Functional Theory. Journal of Physical Chemistry A, 2009, 113, 13483-13491.	2.5	53
40	A two dimensional Heusler alloy model. Solid State Communications, 2009, 149, 73-77.	1.9	2
41	Stability, magnetic behavior, and chemical order of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:msub><mml:mrow Physical Review B, 2009, 79, .	3.2	40
42	Bimetallic Feâ^'Ni Cluster Alloys:â€‰ Stability of Core(Fe)â^'Shell(Ni) Arrays and Their Role Played in the Structure and Magnetic Behavior. Journal of Physical Chemistry C, 2008, 112, 6729-6739.	3.1	20
43	A density-functional study of the structures, binding energies and magnetic moments of the clusters Mo_N(N = 2â€“13), Mo₁₂Fe, Mo₁₂Co and Mo₁₂Ni. Nanotechnology, 2008, 19, 145704.	2.6	24
44	Comparativeab initiostudy of the structural, electronic, and magnetic trends of isoelectronic late<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:math>and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>4</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:math>transition metal clusters. Physical Review B, 2008, 78, .	3.2	59
45	Metallic behavior of Pd atomic clusters. Nanotechnology, 2007, 18, 365706.	2.6	18
46	Magnetic properties of Pd atomic clusters from different theoretical approaches. European Physical Journal D, 2007, 44, 125-131.	1.3	26
47	Magnetic properties of small3dand4dtransition metal clusters: The role of a noncompact growth. Physical Review B, 2006, 73, .	3.2	27
48	Collinear versus noncollinear magnetic order in Pd atomic clusters:Ab initiocalculations. Physical Review B, 2006, 74, .	3.2	15
49	Theoretical investigation of free-standing CoPd nanoclusters as a function of cluster size and stoichiometry in the Pd-rich phase: Geometry, chemical order, magnetism, and metallic behavior. Physical Review B, 2006, 74, .	3.2	52
50	Tight-binding and evolutionary search approach for nanoscale CoRh alloys. Physica B: Condensed Matter, 2005, 370, 200-214.	2.7	13
51	Twining effects in the magnetism of small Pd clusters. Solid State Communications, 2005, 133, 573-578.	1.9	13
52	Structural and magnetic properties of CoRh nanoparticles. Physical Review B, 2004, 70, .	3.2	24
53	Axial anisotropic effects in hysteresis ofÂ±JIsing lattices. Physical Review B, 2004, 70, .	3.2	2
54	Magnetic behavior of Pd nanoclusters. Physica B: Condensed Matter, 2004, 354, 271-277.	2.7	6

#	Article	IF	Citations
55	Magnetic trends in Mnn nanoclusters effects of uniform relaxations on the magnetic properties. Physics Letters, Section A: General, Atomic and Solid State Physics, 2004, 325, 144-148.	2.1	1
56	Magnetic behaviour of selected geometries of Pd clusters: icosahedral versus fcc structures. Physics Letters, Section A: General, Atomic and Solid State Physics, 2004, 330, 126-130.	2.1	11
57	Magnetism in small Pd clusters. Physics Letters, Section A: General, Atomic and Solid State Physics, 2004, 332, 107-114.	2.1	17
58	Magnetism in segregated bimetallic CoRh nanoclusters. Physica B: Condensed Matter, 2004, 354, 278-281.	2.7	4
59	Hysteresis for anisotropic Â±J Ising square lattices. Journal of Alloys and Compounds, 2004, 369, 55-57.	5.5	5
60	Magnetic properties of small vanadium clusters. Journal of Alloys and Compounds, 2004, 369, 52-54.	5.5	3
61	Magnetic structure of cobalt clusters. Journal of Alloys and Compounds, 2004, 369, 93-96.	5.5	11
62	Magnetism in Rh clusters under hydrostatic deformations. European Physical Journal D, 2003, 23, 343-349.	1.3	5
63	Effects of the structural deformations on the magnetism of Rh6 and Rh13 clusters. Physics Letters, Section A: General, Atomic and Solid State Physics, 2003, 318, 473-479.	2.1	4
64	Order parameters in anisotropic two-dimensional Â±J Ising lattices. Physica A: Statistical Mechanics and Its Applications, 2003, 327, 477-490.	2.6	2
65	Magnetism of small Mn clusters. Physica Status Solidi (B): Basic Research, 2003, 239, 457-462.	1.5	6
66	Structure and magnetism of cobalt clusters. Physical Review B, 2003, 67, .	3.2	128
67	Structure and magnetism of small rhodium clusters. Physical Review B, 2002, 66, .	3.2	96
68	Electronic structure and stability of polycrystalline cobalt clusters. Physical Review B, 2002, 65, .	3.2	17
69	Deformation Effects in the Magnetic Moments of Ni Clusters. , 2001, , 77-85.		1
70	Magnetic moments in Ni clusters with deformations. Solid State Communications, 2001, 117, 477-482.	1.9	4
71	Electronic Properties of Small Free Co Clusters. Physica Status Solidi (B): Basic Research, 2000, 220, 455-460.	1.5	4
72	Magnetic interactions between small Ni clusters. Solid State Communications, 2000, 116, 309-314.	1.9	0

#	Article	IF	Citations
73	Nonmetalâ€“metal transition in RhN and RuN clusters. Physics Letters, Section A: General, Atomic and Solid State Physics, 2000, 265, 116-121.	2.1	4
74	Average magnetization and local magnetic moments ofFeNclusters(N<230). Physical Review B, 1999, 60, 434-439.	3.2	43
75	Structural evolution of free Co cluster magnetism. Solid State Communications, 1999, 111, 335-340.	1.9	24
76	Cluster variation method and Monte Carlo simulations in Ising square antiferromagnets. Solid State Communications, 1999, 112, 437-441.	1.9	20
77	On the metallic behavior of Co clusters. Solid State Communications, 1999, 113, 147-151.	1.9	4
78	Magnetic moments of. European Physical Journal D, 1999, 6, 235.	1.3	15
79	Electronic and geometrical effects on the magnetism of small RuN clusters. Journal of Magnetism and Magnetic Materials, 1998, 186, 214-222.	2.3	20
80	Geometrical structure and magnetism of nickel clusters. Solid State Communications, 1998, 107, 25-30.	1.9	13
81	Finite-size effects on the phase diagrams of binary alloy films. Solid State Communications, 1998, 107, 285-289.	1.9	4
82	Magnetic moments of iron clusters: a simple theoretical model. Physics Letters, Section A: General, Atomic and Solid State Physics, 1998, 242, 255-260.	2.1	18
83	Magnetic moments of Ni clusters. Physical Review B, 1998, 57, 12469-12475.	3.2	73
84	Theoretical Study of the Metal-Nonmetal Transition in Transition Metal Clusters. , 1998, , 109-117.		1
85	Magnetic Surface Enhancement and the Curie Temperature in Ising Thin Films. , 1998, , 219-226.		0
86	Phase Transitions in Ising Square Antiferromagnets: A Controversial System. , 1998, , 203-207.		0
87	DIRECT ENUMERATION OF THE GEOMETRICAL CHARACTERISTICS OF CLUSTERS. Scripta Materialia, 1997, 8, 269-287.	0.5	128
88	Nonmetal-metal transition in Ni clusters. Solid State Communications, 1997, 104, 635-639.	1.9	18
89	Cluster Variation Method Applications to Large Ising Aggregates. , 1996, , 219-235.		0
90	Phase transitions in bcc(110) binary-alloy thin films. Physical Review B, 1995, 52, 5392-5399.	3.2	16

#	Article	IF	Citations
91	Magnetic properties of large Ising clusters. Surface Science, 1995, 326, 150-160.	1.9	7
92	Phase transitions in Ising square antiferromagnets with first- and second-neighbour interactions. Journal of Physics Condensed Matter, 1994, 6, 9759-9772.	1.8	34
93	The Pair Approximation of the Cluster Variation Method as Applied to bcc Alloys. Progress of Theoretical Physics Supplement, 1994, 115, 165-169.	0.1	1
94	Finite size scaling in Ising thin films. Solid State Communications, 1994, 91, 435-438.	1.9	10
95	Modeling the magnetic properties of Heusler alloys. Journal of Magnetism and Magnetic Materials, 1994, 131, 417-426.	2.3	30
96	Adsorption of random copolymer on surfaces. Journal De Physique II, 1994, 4, 1651-1675.	0.9	5
97	Mean Field Study of Size Scaling in Ising Thin Films. , 1994, , 167-174.		0
98	Magnetic Properties of Cubo-Octahedral Ising Clusters. , 1994, , 47-55.		0
99	Magnetic properties of cubo-octahedral Ising clusters. Solid State Communications, 1993, 88, 101-104.	1.9	9
100	The s and p character of the electronic structure of C20, C60 and C70. Solid State Communications, 1993, 85, 767-771.	1.9	9
101	Polymer statistics. Physica A: Statistical Mechanics and Its Applications, 1993, 195, 53-73.	2.6	6
102	Electronic structure of some semiconductor fullerenes. Scripta Materialia, 1993, 3, 469-477.	0.5	5
103	Specific heat and the phase diagram of the Ising square lattice with nearest- and next-nearest interactions. Journal of Physics Condensed Matter, 1993, 5, A195-A196.	1.8	11
104	Recursion method study of the electronic structure of some fullerenes. Journal of Physics Condensed Matter, 1993, 5, A389-A392.	1.8	0
105	First-order phase transitions in the Ising square lattice with first- and second-neighbor interactions. Physical Review B, 1993, 48, 3519-3522.	3.2	62
106	End effects in adsorption of homopolymers and triblock copolymers. Journal De Physique II, 1993, 3, 1141-1159.	0.9	1
107	Phase transitions in layered magnetic structures. Solid State Communications, 1992, 82, 71-74.	1.9	5
108	Polymer statistics. Physica A: Statistical Mechanics and Its Applications, 1992, 189, 81-107.	2.6	11

#	Article	IF	Citations
109	Polymer statistics. Physica A: Statistical Mechanics and Its Applications, 1992, 189, 108-126.	2.6	11
110	Polymer statistics. Physica A: Statistical Mechanics and Its Applications, 1992, 182, 331-345.	2.6	12
111	Phase Transitions in Ultrathin Films. Springer Proceedings in Physics, 1992, , 453-462.	0.2	0
112	Polymer statistics. Physica A: Statistical Mechanics and Its Applications, 1991, 176, 514-533.	2.6	11
113	Ising model of phase transitions in ultrathin films. Solid State Communications, 1990, 74, 155-158.	1.9	96
114	Theory of phase equilibria in Co-Fe alloys. Physical Review B, 1985, 31, 1686-1688.	3.2	20
115	Mean-field theory of magnetic transitions in semi-infinite Ising models. Physical Review B, 1985, 31, 7146-7150.	3.2	41
116	Spatial and magnetic ordering of systems chemisorbed at the surface of ferromagnets. Physical Review B, 1984, 30, 2666-2670.	3.2	1
117	Magnetic long- and short-range order at the surface of ferromagnets. Physical Review B, 1983, 28, 3909-3913.	3.2	11