Andrs Vega

List of Publications by Citations

172 papers	2,644 citations	27 h-index	41 g-index
174 ext. papers	2,781 ext. citations	3.2 avg, IF	4.85 L-index

#	Paper	IF	Citations
172	Structure and magnetism of cobalt clusters. *Physical Review B*, **2003**, 67,	3.3	119
171	Structure and magnetism of small rhodium clusters. *Physical Review B*, **2002**, 66,	3.3	93
170	Systematic ab initio study of the electronic and magnetic properties of different pure and mixed iron systems. *Physical Review B*, **2000**, 61, 13639-13646	3.3	93
169	Calculated sp-electron and spd-hybridization effects on the magnetic properties of small FeN clusters. *Physical Review B*, **1993**, 47, 4742-4746	3.3	87
168	Spin polarization at the Fe/V interface. *Physical Review B*, **1993**, 48, 985-992	3.3	68
167	Magnetic moments of Ni clusters. *Physical Review B*, **1998**, 57, 12469-12475	3.3	67
166	Comparative ab initio study of the structural, electronic, and magnetic trends of isoelectronic late 3d and 4d transition metal clusters. *Physical Review B*, **2008**, 78,	3.3	56
165	Structural and magnetic properties of X12Y (X, Y=Fe, Co, Ni, Ru, Rh, Pd, and Pt) nanoalloys. *Journal of Chemical Physics*, **2010**, 132, 184507	3.9	53
164	Antiferromagnetic interlayer coupling in Fe/V and Fe/Cr. *Journal of Applied Physics*, **1991**, 69, 4544-4546	2.5	52
163	Ti-decorated zigzag graphene nanoribbons for hydrogen storage. A van der Waals-corrected density-functional study. *International Journal of Hydrogen Energy*, **2015**, 40, 4960-4968	6.7	48
162	Geometrical effects on the magnetism of small Ni clusters. *Physical Review B*, **1997**, 55, 13279-13282	3.3	47
161	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,	3.3	46
160	Study of the structural and electronic properties of Rh(N) and Ru(N) clusters (N Journal of Physical Chemistry A, **2009**, 113, 13483-91	2.8	45
159	Induced spin polarization in V:FenVm superlattices and thin V films on Fe substrates. *Physical Review B*, **1999**, 59, 14510-14515	3.3	39
158	Average magnetization and local magnetic moments of FeN clusters (N. *Physical Review B*, **1999**, 60, 434-439	3.3	39
157	Possibility of various magnetic configurations in the Cr (Fe) monolayer deposited on vicinal surfaces of Fe (Cr). *Physical Review B*, **1995**, 51, 11546-11554	3.3	38
156	Topological antiferromagnetism at Cr surfaces and interfaces. *Physical Review B*, **1994**, 49, 12797-12800	3.3	36

155	Stability, magnetic behavior, and chemical order of (CoxFe1□)N (N=5,13) nanoalloys. *Physical Review B*, **2009**, 79,	3.3	35
154	All-electron and pseudopotential study of the spin-polarization of the V(001) surface: LDA versus GGA. *Physical Review B*, **2001**, 63,	3.3	34
153	Noncollinear Fe spin structure in (Sm-Co)/Fe exchange-spring bilayers: Layer-resolved 57Fe M□ssbauer spectroscopy and electronic structure calculations. *Physical Review B*, **2012**, 85,	3.3	31
152	Noncollinear magnetism of thin Cr films deposited on a stepped Fe (001) surface. *Physical Review B*, **2003**, 68,	3.3	31
151	Magnetic and electronic properties of substitutional FeN cluster impurities in Cr: Transition from antiferromagnetic to ferromagnetic FeN. *Physical Review B*, **1994**, 50, 3899-3906	3.3	31
150	Magnetism of Co nanoparticles supported on the Cu(111) substrate: Size and environment dependence. *Physical Review B*, **1997**, 55, 445-451	3.3	29
149	Magnetic-Order Transition in Thin Fe Overlayers on Cr: Role of the Interfacial Roughness. *Europhysics Letters*, **1995**, 31, 561-566	1.6	29
148	What will freestanding borophene nanoribbons look like? An analysis of their possible structures, magnetism and transport properties. *Physical Chemistry Chemical Physics*, **2017**, 19, 1054-1061	3.6	28
147	Optical properties of large band gap □n2S3□xO3x compounds obtained by physical vapour deposition. *Optical Materials*, **2005**, 27, 647-653	3.3	28
146	Hydrogen Interaction in Pd□t Alloy Nanoparticles. *Journal of Physical Chemistry C*, **2012**, 116, 126-133	3.8	27
145	Antiferromagnetic interlayer coupling in Fe/c-SiFe/Fe sandwiches and multilayers. *Physical Review B* , **2001**, 65,	3.3	26
144	Electronic quasiparticle structure of ferromagnetic bcc iron. *European Physical Journal B*, **1995**, 96, 357-372	1.2	26
143	Ab initio study of the adsorption of NO on the Rh6(+) cluster. *Journal of Physical Chemistry A*, **2011**, 115, 8350-60	2.8	25
142	Magnetic properties of Pd atomic clusters from different theoretical approaches. *European Physical Journal D*, **2007**, 44, 125-131	1.3	25
141	Origin of dead magnetic Fe overlayers on V(110). *Physical Review B*, **2001**, 64,	3.3	25
140	C(2 □2) ferrimagnetic order versus P(1 □1) ferromagnetic order in V, Cr, Mn monolayers on Fe(001). *Thin Solid Films*, **1996**, 275, 103-105	2.2	25
139	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	3.9	24
138	Al enhances the H2 storage capacity of graphene at nanoribbon borders but not at central sites: A study using nonlocal van der Waals density functionals. *Physical Review B*, **2012**, 85,	3.3	24

137	Structural and magnetic properties of CoRh nanoparticles. *Physical Review B*, **2004**, 70,	3.3	24
136	Spin configuration in a frustrated ferromagnetic/antiferromagnetic thin-film system. *Nanotechnology*, **2007**, 18, 235702	3.4	23
135	Magnetic behavior of monoatomic Co wires on Pd(110). *Physical Review B*, **2000**, 61, 6848-6853	3.3	23
134	Self-consistent theory of overlap interactions in the tight-binding method. *Physical Review B*, **1993**, 47, 12995-12998	3.3	23
133	Structural and zero-point vibrational effects on the electric dipole moments and static dipole polarizabilities of sodium clusters. *Physical Review B*, **2011**, 84,	3.3	22
132	Structure, fragmentation patterns, and magnetic properties of small cobalt oxide clusters. *Physical Chemistry Chemical Physics*, **2014**, 16, 21732-41	3.6	21
131	Insulating or metallic: coexistence of different electronic phases in zinc clusters. *Angewandte Chemie - International Edition*, **2015**, 54, 2111-5	16.4	21
130	Tight-binding study of the ionization of iron clusters. *Physical Review B*, **1996**, 54, 3003-3006	3.3	21
129	A density-functional study of the possibility of noncollinear magnetism in small Mn clusters using SIESTA and the generalized gradient approximation to exchange and correlation. *Journal of Chemical Physics*, **2008**, 128, 114315	3.9	20
128	Finite-temperature ferromagnetism of f.c.c. cobalt. *Physica Status Solidi (B): Basic Research*, **1996**, 193, 177-187	1.3	20
127	Li-decorated Pmmn8 phase of borophene for hydrogen storage. A van der Waals corrected density-functional theory study. *International Journal of Hydrogen Energy*, **2019**, 44, 1021-1033	6.7	20
126	Tailoring the spin density waves in Fe/Cr multilayers by selective inclusion of Sn, V and Mn. *Surface Science*, **2009**, 603, 117-124	1.8	19
125	A density-functional study of the structures, binding energies and magnetic moments of the clusters Mo(N) (N = 2-13), Mo(12)Fe, Mo(12)Co and Mo(12)Ni. *Nanotechnology*, **2008**, 19, 145704	3.4	19
124	Magnetic magic numbers are not magic for clusters embedded in noble metals. *Physical Review B*, **2002**, 66,	3.3	19
123	Molecular hydrogen uptake by zigzag graphene nanoribbons doped with early 3d transition-metal atoms. *International Journal of Hydrogen Energy*, **2013**, 38, 8872-8880	6.7	17
122	Density functional study of ternary Fe x Co y Ni z (x + y + z = 7) clusters. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	17
121	Nonmetal-metal transition in Ni clusters. *Solid State Communications*, **1997**, 104, 635-639	1.6	17
120	Competition between two- and three-dimensional growth of Co clusters deposited on Cu(001): Influence on the magnetic properties. *Physical Review B*, **2001**, 63,	3.3	17

119	Magnetism of Vicinal Surfaces of Vanadium. *Europhysics Letters*, **1994**, 27, 165-170	1.6	17
118	Magnetic properties of semi-infinite systems of Cr(Fe) on a Fe(Cr) (001) surface. *Surface Science*, **1991**, 251-252, 51-54	1.8	17
117	Structure and magnetic properties of small Fe clusters supported on the Ni(001) surface. *Physical Review B*, **2005**, 71,	3.3	16
116	Magnetism in small Pd clusters. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2004**, 332, 107-114	2.3	16
115	Collinear versus noncollinear magnetic order in Pd atomic clusters: Ab initio calculations. *Physical Review B*, **2006**, 74,	3.3	15
114	Stepped Fe(001) surface magnetism. *Journal of Magnetism and Magnetic Materials*, **1992**, 104-107, 1687-1688	1.6	15
113	Magnetic moments of. *European Physical Journal D*, **1999**, 6, 235	1.3	15
112	A new magnetic superatom: Cr@Zn *Physical Chemistry Chemical Physics*, **2015**, 17, 28033-43	3.6	14
111	Structural, electronic, and magnetic properties Of Co(n)Cu(m) nanoalloys (m + n = 12) from first principles calculations. *Journal of Physical Chemistry A*, **2012**, 116, 9353-60	2.8	14
110	The magnetization reversal process in spin spring magnets. *Nanotechnology*, **2008**, 19, 315401	3.4	14
109	Metallic behavior of Pd atomic clusters. *Nanotechnology*, **2007**, 18, 365706	3.4	14
108	Optical conductivity in substoichiometric titanium carbides. *Physical Review B*, **1998**, 58, 3507-3510	3.3	14
107	Mo4 Fex nanoalloy: Structural transition and electronic structure of interest in spintronics. *Physical Review B*, **2009**, 79,	3.3	13
106	Engineering the magnetic structure of Fe clusters by Mn alloying. *Nanotechnology*, **2008**, 19, 245701	3.4	13
105	Twining effects in the magnetism of small Pd clusters. *Solid State Communications*, **2005**, 133, 573-578	1.6	13
104	Antiferromagnetic versus ferromagnetic orders in V, Cr and Mn overlayers on Fe(103). *Journal of Magnetism and Magnetic Materials*, **1995**, 148, 177-178	2.8	13
103	Hydrogen insertion in Pd core/Pt shell cubo-octahedral nanoparticles. *Physical Review B*, **2011**, 83,	3.3	12
102	Impact of dimerization and stretching on the transport properties of molybdenum atomic wires. *Nanotechnology*, **2010**, 21, 095205	3.4	12

101	Multiple collinear magnetic arrangements in thin Mn films supported on Fe(001). Antiferromagnetic versus ferromagnetic behavior. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2005**, 337, 469-472	2.3	12
100	Tight-binding and evolutionary search approach for nanoscale CoRh alloys. *Physica B: Condensed Matter*, **2005**, 370, 200-214	2.8	12
99	Ab initio optical conductivity in LaMO3 (M=Ti-Cu). *Physical Review B*, **1996**, 54, 11271-11275	3.3	12
98	Spin-polarized transport in hydrogen-passivated graphene and silicene nanoribbons with magnetic transition-metal substituents. *Physical Chemistry Chemical Physics*, **2016**, 18, 22606-16	3.6	11
97	Structural and magnetic properties of Fen clusters at the Al (001) surface: Early transition from paramagnetic to ferromagnetic Fen. *Physical Review B*, **2004**, 69,	3.3	11
96	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	2.3	11
95	Magnetic structure of cobalt clusters. *Journal of Alloys and Compounds*, **2004**, 369, 93-96	5.7	11
94	Unusual effect of interatomic interactions on magnetism: Rh adatoms on the Ag(001) surface. *Physical Review B*, **1998**, 57, R14020-R14023	3.3	11
93	Antiferromagnetic-like coupling in the cationic iron cluster of thirteen atoms. *Physical Chemistry Chemical Physics*, **2013**, 15, 14458-64	3.6	10
92	Density functional study of the optical response of FeN and CoN nitrides with zinc-blend and rock-salt structures. *Journal of Physics and Chemistry of Solids*, **2017**, 100, 148-153	3.9	10
91	A new family of star-like icosahedral structures for small cobalt clusters. *Chemical Physics*, **2013**, 415, 106-111	2.3	10
90	Magnetic cooperative effects in small Ni-Ru clusters. *Journal of Physical Chemistry A*, **2011**, 115, 13950-5	2.8	10
89	Magnetic moments of Ni monolayers and small ground-state Ni clusters at the Al (001) surface. *Physical Review B*, **2000**, 62, 11104-11108	3.3	10
88	On the electric dipole moments of small sodium clusters from different theoretical approaches. *Chemical Physics*, **2012**, 399, 252-257	2.3	9
87	Density functional study of the structures and electronic properties of nitrogen-doped Ni(n) clusters, n = 1-10. *Journal of Physical Chemistry A*, **2011**, 115, 13997-4005	2.8	9
86	Theoretical study of the gap evolution of In2X3 (X=O, S, Se, Te) with lattice compression. *Optical Materials*, **2001**, 17, 497-499	3.3	9
85	Vanadium: From cluster to semi-infinite crystal. *Journal of Applied Physics*, **1993**, 73, 6207-6209	2.5	9
84	New structural and electronic properties of (TiO2)10. *Journal of Chemical Physics*, **2016**, 144, 234312	3.9	9

83	Density Functional Study of Charge Transfer at the Graphene/Ionic Liquid Interface. *Journal of Physical Chemistry C*, **2018**, 122, 15070-15077	3.8	9
82	Theoretical study of Al(n)V+ clusters and their interaction with Ar. *Journal of Chemical Physics*, **2013**, 139, 214305	3.9	8
81	Interplay between structure and magnetism in hydride iron-vanadium systems. *Physical Review B*, **2008**, 78,	3.3	8
80	Possibility of collinear magnetic order in frustrated free-standing Fe2Cr4 clusters. *Physical Review B*, **2008**, 77,	3.3	8
79	Electronic structure calculations of low-dimensional transition metals. *Handbook of Magnetic Materials*, **2003**, 15, 199-288	1.3	8
78	Calculation of electronic properties of the (100) surface of Fe including overlap interactions. *Surface Science*, **1991**, 251-252, 55-58	1.8	8
77	Structural and electronic properties of TM(n)[(BN)(3)H(6)](m) complexes with TM = Co (n, m = 1-3) and with TM = Fe, Ni, Ru, Rh, Pd (n = m = 1-3). *Journal of Physical Chemistry A*, **2014**, 118, 2976-83	2.8	7
76	Insulating or Metallic: Coexistence of Different Electronic Phases in Zinc Clusters. *Angewandte Chemie*, **2015**, 127, 2139-2143	3.6	7
75	Zn17 Superatom Cage Doped with 3d Transition-Metal (TM) Impurities (TM = Sc, Ti, V, Cr, Mn, Fe, Co, Ni, and Cu). *Journal of Physical Chemistry C*, **2015**, 119, 27838-27847	3.8	7
74	Structure and electronic properties of molybdenum monatomic wires encapsulated in carbon nanotubes. *Journal of Physics Condensed Matter*, **2011**, 23, 265302	1.8	7
73	A density-functional study of the structures and electronic properties of neutral, anionic, and endohedrally doped In(x)P(x) clusters. *Journal of Chemical Physics*, **2009**, 131, 074504	3.9	7
72	Noncollinear magnetism caused by intermixing at ferromagnetic/antiferromagnetic interfaces. *Physical Review B*, **2006**, 74,	3.3	7
71	Is the vanadium(001) surface magnetic? Pseudopotential toward all-electron calculations. *International Journal of Quantum Chemistry*, **2003**, 91, 230-233	2.1	7
70	Borophene vs. graphene interfaces: Tuning the electric double layer in ionic liquids. *Journal of Molecular Liquids*, **2020**, 303, 112647	6	7
69	Are zinc clusters really amorphous? A detailed protocol for locating global minimum structures of clusters. *Nanoscale*, **2018**, 10, 19162-19181	7.7	7
68	Properties Design: Prediction and Experimental Validation of the Luminescence Properties of a New Eu -Based Phosphor. *Chemistry - A European Journal*, **2018**, 24, 16276-16281	4.8	7
67	Structural, Electronic, and Magnetic Properties of Iron Disulfide FeS (n = 1-6) Clusters. *Journal of Physical Chemistry A*, **2017**, 121, 3768-3780	2.8	6
66	Nanoscale reactivity of ZnxMg20⊠ investigated by structural and electronic indicators. *Corrosion Science*, **2017**, 124, 35-45	6.8	6

65	Structure, fragmentation patterns, and magnetic properties of small nickel oxide clusters. *Physical Chemistry Chemical Physics*, **2017**, 19, 3366-3383	3.6	6
64	Density functional study of the structural, electronic, and magnetic properties of Mo n and Mo n S (n = 1 10) clusters. *Journal of Nanoparticle Research*, **2017**, 19, 1	2.3	6
63	Electronic structure and transport properties of monatomic Fe chains in a vacuum and anchored to a graphene nanoribbon. *Journal of Physics Condensed Matter*, **2012**, 24, 455304	1.8	6
62	Spin polarization at Fe/Cr interfaces. *Journal of Applied Physics*, **1997**, 81, 4347-4349	2.5	6
61	Interlayer exchange coupling in Fe/SiFe/Fe sandwiches. *Surface Science*, **2001**, 482-485, 994-997	1.8	6
60	Onset of C(2) ferrimagnetic order in Cr islands deposited on Fe(001) as a function of island size. *Journal of Applied Physics*, **1996**, 79, 5834	2.5	6
59	Spin-polarization of thin Mn films on Fe(107). *Journal of Magnetism and Magnetic Materials*, **1996**, 156, 199-201	2.8	6
58	Defects and Magnetic Properties: The Cr/Fe(001) Interfaces. *Materials Research Society Symposia Proceedings*, **1995**, 384, 247		6
57	Spin-orbit effects on the structural, homotop, and magnetic configurations of small pure and Fe-doped Pt clusters. *Journal of Nanoparticle Research*, **2014**, 16, 1	2.3	5
56	Spin-dependent electronic conduction along zigzag graphene nanoribbons bearing adsorbed Ni and Fe nanostructures. *Journal of Physics Condensed Matter*, **2014**, 26, 165302	1.8	5
55	Electronic structure investigation of the exchange-spring behavior during the magnetic reversal process. *Physical Review B*, **2008**, 77,	3.3	5
54	Magnetic behavior of Pd nanoclusters. *Physica B: Condensed Matter*, **2004**, 354, 271-277	2.8	5
53	Magnetic properties of Co islands grown on Cu(111). *Surface Science*, **1996**, 352-354, 902-906	1.8	5
52	Impact of S doping on the structural, electronic and magnetic properties of Cr n (n = 2 6) clusters. *European Physical Journal D*, **2017**, 71, 1	1.3	4
51	Improvement of hydrogen uptake in iron and vanadium matrices by doping with 3d atomic impurities. *Journal of Alloys and Compounds*, **2012**, 545, 19-27	5.7	4
50	Charge and spin transport properties of Mo2X2 (X = Fe,Co,Ni) molecular contacts. *Physical Review B* , **2012**, 85,	3.3	4
49	Magnetism in segregated bimetallic CoRh nanoclusters. *Physica B: Condensed Matter*, **2004**, 354, 278-281	2.8	4
48	Magnetism in Rh clusters under hydrostatic deformations. *European Physical Journal D*, **2003**, 23, 343-349	2.3	4

47	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	2.3	4
46	Theoretical study of the charge transfer in supported transition metal microclusters. *European Physical Journal D*, **2005**, 34, 51-54	1.3	4
45	Antiferromagnetic versus ferromagnetic coupling in Fe/Cr(107) and Cr/Fe(107). *Journal of Applied Physics*, **1994**, 76, 6989-6991	2.5	4
44	Geometrical and chemical environment effects on the magnetism of stepped surfaces of V and V over Fe. *European Physical Journal D*, **1993**, 43, 1045-1050		4
43	Predicting photon cascade emission in Pr doped fluorides. *Physical Chemistry Chemical Physics*, **2017** , 19, 15503-15511	3.6	3
42	Spin currents and filtering behavior in zigzag graphene nanoribbons with adsorbed molybdenum chains. *Journal of Physics Condensed Matter*, **2015**, 27, 135301	1.8	3
41	Structural, Vibrational, and Magnetic Properties of FeCoOn0/+ (n = 1) Bimetallic Oxide Clusters. *Journal of Physical Chemistry C*, **2015**, 119, 11200-11209	3.8	3
40	Ab initio study of hydrogen insertion in ultrathin transition metal doped V films: Structural and electronic properties. *Physical Review B*, **2010**, 81,	3.3	3
39	Response of Mn overlayers on Fe to external magnetic fields: Electronic structure calculations. *Surface Science*, **2009**, 603, 2537-2543	1.8	3
38	The structure of an Fe monolayer on the Ni (111) surface. A density-functional study using the generalized gradient approximation. *Solid State Communications*, **2006**, 137, 129-131	1.6	3
37	Magnetic coupling in the cluster Fe2Mn4 : A fully unconstrained density-functional study. *Solid State Communications*, **2006**, 140, 480-482	1.6	3
36	Temperature-dependent magnetic behavior of ideal and stepped Fe surfaces. *Physical Review B*, **2001**, 63,	3.3	3
35	Electronic structure and optical response of L-CePd5. *Physical Review B*, **1995**, 51, 4823-4829	3.3	3
34	Optical absorption and interband transitions in CePd7. *Physical Review B*, **1996**, 53, 6881-6884	3.3	3
33	Magnetic properties of very thin V films adsorbed on Fe substrate. *Journal of Magnetism and Magnetic Materials*, **1993**, 121, 177-179	2.8	3
32	Incorporating charge transfer effects into a metallic empirical potential for accurate structure determination in (ZnMg) nanoalloys. *Nanoscale*, **2020**, 12, 20432-20448	7.7	3
31	Structural and Electronic Rearrangements in FeS, FeS, and FeS Atomic Clusters under the Attack of NO, CO, and O. *Journal of Physical Chemistry A*, **2019**, 123, 10919-10929	2.8	3
30	Hydrogen storage capacity of Li-decorated borophene and pristine graphene slit pores: A combined ab initio and quantum-thermodynamic study. *Applied Surface Science*, **2021**, 562, 150019	6.7	3

29	Structural, magnetic, and vibrational properties of stoichiometric clusters of CrN. *International Journal of Quantum Chemistry*, **2015**, 115, 523-528	2.1	2
28	Proximity effects on the spin density waves in X/Cr(001) multilayers (X=Sn, V, and Mn). *Thin Solid Films*, **2011**, 519, 2037-2042	2.2	2
27	Magnetization reversal process at atomic scale in systems with itinerant electrons. *Journal of Physics Condensed Matter*, **2012**, 24, 176002	1.8	2
26	Magnetic moments in Ni clusters with deformations. *Solid State Communications*, **2001**, 117, 477-482	1.6	2
25	Small Ni clusters at the (1 1 0) and (1 1 1) surfaces of Al: structures and lack of magnetic moment. *Surface Science*, **2001**, 482-485, 976-980	1.8	2
24	Structure, fragmentation patterns, and electronic properties of small indium oxide clusters. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	1
23	Titanium embedded cage structure formation in Al(n)Ti+ clusters and their interaction with Ar. *Journal of Chemical Physics*, **2014**, 140, 174304	3.9	1
22	Response of magnetically frustrated nanostructures to external magnetic fields: Stepped Cr/Fe interfaces. *Physical Review B*, **2010**, 81,	3.3	1
21	Electronic, magnetic, and optical properties of. *Journal of Physics Condensed Matter*, **1997**, 9, 6267-6277	1.8	1
20	Competition between CoCr hybridization and low-coordination effects in the magnetism of a Co monolayer deposited on Cr substrates. *Journal of Magnetism and Magnetic Materials*, **1997**, 165, 265-267	2.8	1
19	Morphology and magnetism of Fe monolayers and small Fenclusters (n= 2□9) supported on the Ni(111) surface. *Nanotechnology*, **2007**, 18, 055701	3.4	1
18	Magnetism of the Fe9 nanocluster supported on Ni(001). *Computational Materials Science*, **2006**, 35, 307-310	3.2	1
17	Deformation Effects in the Magnetic Moments of Ni Clusters **2001**, 77-85		1
16	Magnetic properties of small 3-d transition metal clusters: Role of the sp-electrons and spd-hybridization. *Scripta Materialia*, **1993**, 3, 359-363		1
15	Calculation of the magnetic properties of FeN clusters embedded in 3d transition-metal matrices. *Computational Materials Science*, **1994**, 2, 463-467	3.2	1
14	Stepped Fe(100) and V/Fe(100) Magnetism. *Materials Research Society Symposia Proceedings*, **1991**, 231, 323		1
13	Ab initio study of lithium decoration of popgraphene and hydrogen storage capacity of the hybrid nanostructure. *International Journal of Hydrogen Energy*, **2021**, 46, 15724-15737	6.7	1
12	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	3.6	1

List of Publications

11	A neural network potential for searching the atomic structures of pure and mixed nanoparticles. Application to ZnMg nanoalloys with an eye on their anticorrosive properties. *Acta Materialia*, **2021**, 220, 117341	8.4	1
10	Why are Zn-rich Zn-Mg nanoalloys optimal protective coatings against corrosion? A first-principles study of the initial stages of the oxidation process. *Physical Chemistry Chemical Physics*, **2021**, 23, 24685-24698	3.6	0
9	Interfacial effects on the magnetic profiles and interlayer exchange coupling of Co/CoSi multilayers. *Thin Solid Films*, **2011**, 520, 302-306	2.2	
8	Temperature dependent magnetic behaviour of thin Fe(0 0 1) films with 1.5, 2, 2.5 and 3 monolayers. *Surface Science*, **2005**, 582, 209-214	1.8	
7	NON-COLLINEAR MAGNETISM IN THE Fe3 MICROCLUSTER: FREE-STANDING VS SUPPORTED ENVIRONMENTS. *International Journal of Modern Physics B*, **2005**, 19, 2532-2537	1.1	
6	Magnetic interactions between small Ni clusters. *Solid State Communications*, **2000**, 116, 309-314	1.6	
5	Temperature-dependent magnetic behavior of the Fe (100) surface. *Computational Materials Science*, **2000**, 17, 473-476	3.2	
4	Theoretical study of induced V polarization at the interface with Fe in Fe n V m superlattices. *The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties*, **1998**, 78, 469-473		
3	C(2 □2) ferrimagnetic order versus p(1 □1) ferromagnetic order in V, Cr, Mn monolayers on Fe(001) **1996**, 103-105		
2	Structural properties, magnetism and reactivity of Ni13-xFex nanoalloys. *Journal of Magnetism and Magnetic Materials*, **2021**, 524, 167636	2.8	
1	Unveiling the effects of doping small nickel clusters with a sulfur impurity. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	