Luis C BalbÃ¡s

List of Publications by Year
in descending order

128 papers	3,135 citations	172207 29 h-index	174990 52 g-index
129 all docs	129 docs citations	129 times ranked	1991 citing authors

#	Article	IF	Citations
1	Trends in the structure and bonding of noble metal clusters. Physical Review B, 2004, 70, .	1.1	509
2	Ab InitioPhotoabsorption Spectra and Structures of Small Semiconductor and Metal Clusters. Physical Review Letters, 1996, 77, 247-250.	2.9	193
3	Planar and cagelike structures of gold clusters: Density-functional pseudopotential calculations. Physical Review B, 2006, 73, .	1.1	108
4	Theoretical study of structural, electronic, and magnetic properties ofAunM+clusters (M=Sc, Ti, V,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	1.1	105
5	Systematicab initiostudy of the electronic and magnetic properties of different pure and mixed iron systems. Physical Review B, 2000, 61, 13639-13646.	1.1	98
6	Theoretical study of O2 and CO adsorption on Aun clusters (n=5â€“10). Chemical Physics Letters, 2005, 408, 252-257.	1.2	95
7	Theoretical study of isoelectronicSinMclusters (M=Scâˆ',Ti,V+;n=14â€“18). Physical Review B, 2007, 75, .	1.1	92
8	Calculatedsp-electron andspd-hybridization effects on the magnetic properties of smallFeNclusters. Physical Review B, 1993, 47, 4742-4746.	1.1	89
9	Spin polarization at the Fe/V interface. Physical Review B, 1993, 48, 985-992.	1.1	69
10	Antiferromagnetic interlayer coupling in Fe/V and Fe/Cr. Journal of Applied Physics, 1991, 69, 4544-4546.	1.1	56
11	Theoretical Study of Oxygen Adsorption on Pure Aun+1+ and Doped MAun+ Cationic Gold Clusters for M = Ti, Fe and n = 3âˆ'7. Journal of Physical Chemistry A, 2008, 112, 6678-6689.	1.1	55
12	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.	1.1	53
13	Ab initio calculations of H2O and O2 adsorption on Al2O3 substrates. Computational Materials Science, 2007, 39, 587-592.	1.4	50
14	Study of the kinetic energy density functional in the locally linear potential approximation. Journal of Chemical Physics, 1985, 83, 5778-5783.	1.2	48
15	Influence of nonlocal exchange-correlation effects on the response properties of simple metal clusters. Physical Review B, 1992, 46, 4891-4898.	1.1	47
16	Density-functional calculation of the fragmentation of doubly ionized spherical jelliumlike metallic microparticles. Physical Review B, 1986, 34, 2152-2157.	1.1	46
17	Response properties of sodium clusters within a jellium-like model with finite surface thickness. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1991, 19, 93-96.	1.0	45
18	Weighted-density exchange and local-density Coulomb correlation energy functionals for finite systems: Application to atoms. Physical Review A, 1993, 48, 4197-4212.	1.0	42

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19	STRUCTURAL PROPERTIES OF BIMETALLIC CLUSTERS FROM DENSITY FUNCTIONAL CALCULATIONS. International Journal of Modern Physics B, 2005, 19, 2339-2344.	1.0	40
20	Static dipole polarizability of alkali-metal clusters: Electronic exchange and correlation effects. Physical Review B, 1990, 42, 10950-10964.	1.1	37
21	Topological antiferromagnetism at Cr surfaces and interfaces. Physical Review B, 1994, 49, 12797-12800.	1.1	36
22	Theoretical study of the stability of AgN2+, AgN, AgN, AgNâ˜' and NaNâ˜' clusters as a function of size using the density functional formalism. Chemical Physics, 1988, 120, 239-247.	0.9	34
23	Theoretical study of the photoabsorption spectrum ofNa8,Na20,Cs8, andCs10O clusters. Physical Review B, 1992, 45, 13657-13663.	1.1	34
24	All-electron and pseudopotential study of the spin-polarization of the V(001) surface: LDA versus GGA. Physical Review B, 2001, 63, .	1.1	34
25	Magnetic and electronic properties of substitutionalFeNcluster impurities in Cr: Transition from antiferromagnetic to ferromagneticFeN. Physical Review B, 1994, 50, 3899-3906.	1.1	32
26	Magic numbers of sodium clusters. Solid State Communications, 1986, 57, 85-88.	0.9	31
27	GGA versus van der Waals density functional results for mixed gold/mercury molecules and pure Au and Hg cluster properties. Physical Chemistry Chemical Physics, 2011, 13, 20863.	1.3	31
28	Magnetism of Co nanoparticles supported on the Cu(111) substrate: Size and environment dependence. Physical Review B, 1997, 55, 445-451.	1.1	29
29	Evaluation of exchange-correlation energy, potential, and stress. Physical Review B, 2001, 64, .	1.1	29
30	Trends in the structure and bonding of neutral and charged noble metal clusters. International Journal of Quantum Chemistry, 2005, 101, 740-745.	1.0	28
31	First-principles calculations of structural and electronic properties of Ta-doped Si clusters, wires, and bulk systems. Physical Review B, 2011, 83, .	1.1	27
32	Study of the Structural and Electronic Properties of [Ti@Si₁₆]_n, [Sc@Si₁₆K]_n, and [V@Si₁₆F]_n (n â‰¤) TjET Qq0 0 0 rgBT /Ov	1.5	27
33	The static polarisability of metal clusters and spheres in an improved Thomas-Fermi approximation. Journal of Physics Condensed Matter, 1989, 1, 10391-10405.	0.7	26
34	Ab Initio Study of the Adsorption of NO on the Rh6+Cluster. Journal of Physical Chemistry A, 2011, 115, 8350-8360.	1.1	25
35	Al enhances the H<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>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, .	1.1	25
36	Structure, fragmentation patterns, and magnetic properties of small cobalt oxide clusters. Physical Chemistry Chemical Physics, 2014, 16, 21732-21741.	1.3	25

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37	Hydrogen Chemisorption on Singly Vanadiumâ€Doped Aluminum Clusters. Chemistry - A European Journal, 2017, 23, 15638-15643.	1.7	24
38	Structural and zero-point vibrational effects on the electric dipole moments and static dipole polarizabilities of sodium clusters. Physical Review B, 2011, 84, .	1.1	23
39	Dissociation channels ofNaN+clusters (3â‰¤Nâ‰¤37). Physical Review B, 1990, 41, 5595-5601.	1.1	22
40	Stability ofNanPb (nâ©½7) clusters: A first-principles molecular-dynamics study. Physical Review B, 1996, 54, 2937-2941.	1.1	22
41	Density functional study of neutral and charged sodium and lead clusters in the jellium model. Physica B: Condensed Matter, 1990, 167, 19-32.	1.3	19
42	Non-local exchange and local Coulomb correlation energy density functionals for finite many-electron systems. Chemical Physics Letters, 1993, 205, 348-353.	1.2	19
43	Nonlocal exchange and kinetic energy density functionals with correct asymptotic behavior for electronic systems. International Journal of Quantum Chemistry, 1994, 49, 171-184.	1.0	19
44	Polarizabilities of aluminium clusters. Solid State Communications, 1990, 75, 139-142.	0.9	18
45	Electronic structure of negatively charged aluminium clusters. Physica B: Condensed Matter, 1991, 168, 32-38.	1.3	18
46	Electronegativity of positive ions in the density functional theory. Zeitschrift FÃ¼r Physik A, 1982, 305, 31-37.	1.4	17
47	Magnetism of Vicinal Surfaces of Vanadium. Europhysics Letters, 1994, 27, 165-170.	0.7	17
48	Relative stability of Sin and SinSc- clusters in the range n = 14â€“18. European Physical Journal D, 2007, 43, 217-220.	0.6	17
49	Trends in the bonding of the first-row transition metal compounds: V(001) surface, TM-oxide and nitride molecules, and Au n Ti (2â‰¤n â‰¤7) clusters. International Journal of Quantum Chemistry, 2004, 99, 39-46.	1.0	16
50	Theoretical study of the structural and electronic properties of aggregates, wires, and bulk phases formed from M@Si₁₆ superatoms (M = Sc^{â^}, Ti, V⁺). International Journal of Quantum Chemistry, 2011, 111, 444-462.	1.0	16
51	One-Electron Energy Eigenvalues in the Weighted-Density Approximation to Exchange and Correlation. Europhysics Letters, 1991, 14, 323-329.	0.7	15
52	Antiferromagnetic-like coupling in the cationic iron cluster of thirteen atoms. Physical Chemistry Chemical Physics, 2013, 15, 14458.	1.3	15
53	X-ray scattering factors of crystalline silicon and germanium from A bond charge model. Journal of Physics and Chemistry of Solids, 1988, 49, 1013-1017.	1.9	14
54	Nonlocal exchange- and kinetic-energy density functionals for electronic systems: Application to atoms and ions. Physical Review A, 1993, 47, 1804-1810.	1.0	14

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55	Self-consistent local-density approximation with model Coulomb pair-correlation functions for electronic systems. Physical Review A, 1993, 47, 1811-1816.	1.0	14
56	Adsorption and dissociation of water on relaxed alumina clusters: a first principles study. Physica Status Solidi (B): Basic Research, 2005, 242, 807-809.	0.7	14
57	Theoretical study of the coadsorption of CO and O2 on doped cationic gold clusters MAun + (M = Ti,) Tj ETQq1 1 0.784314 rgBT /Ove	0.6	14
58	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.	1.1	14
59	Electronegativity equalization and electron transfer in molecules. Molecular Physics, 1983, 48, 981-988.	0.8	13
60	Nonlocal density functional calculation of the electron affinity of atoms. Physics Letters, Section A: General, Atomic and Solid State Physics, 1986, 114, 236-240.	0.9	13
61	New structural and electronic properties of (TiO2)10. Journal of Chemical Physics, 2016, 144, 234312.	1.2	13
62	Local behavior of the kinetic energy in density functional theory. International Journal of Quantum Chemistry, 1985, 27, 393-406.	1.0	12
63	Magnetic properties of 3d-transition-metal alloy clusters: (Fe x Cr1?x) n. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1991, 19, 263-265.	1.0	12
64	Unusual effect of interatomic interactions on magnetism:â€‚Rh adatoms on the Ag(001) surface. Physical Review B, 1998, 57, R14020-R14023.	1.1	12
65	A new family of star-like icosahedral structures for small cobalt clusters. Chemical Physics, 2013, 415, 106-111.	0.9	12
66	Structure, fragmentation patterns, and magnetic properties of small nickel oxide clusters. Physical Chemistry Chemical Physics, 2017, 19, 3366-3383.	1.3	12
67	A non local approximation to the correlation energy of inhomogeneous electron systems. Physics Letters, Section A: General, Atomic and Solid State Physics, 1981, 81, 467-469.	0.9	11
68	Study of an approximate relation between the energy of an atom and the electronic potential at the nucleus. International Journal of Quantum Chemistry, 1982, 22, 989-997.	1.0	11
69	Nonlocal exchange and kinetic-energy density functionals for electronic systems. International Journal of Quantum Chemistry, 1992, 44, 347-358.	1.0	11
70	Pure and Mixed Pb Clusters of Interest for Liquid Ionic Alloys. Advances in Quantum Chemistry, 1998, 33, 329-348.	0.4	11
71	Vanadium: From cluster to semiâ€infinite crystal. Journal of Applied Physics, 1993, 73, 6207-6209.	1.1	10
72	Study of (Al2O3)n(Ox) clusters with n ? 16 and x = 0, 1, 2 from first principles calculations. European Physical Journal D, 2003, 24, 245-248.	0.6	10

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73	Theoretical Study of CO Adsorption on Gold/Alumina Substrates. Journal of Physical Chemistry B, 2006, 110, 10449-10454.	1.2	10
74	Ionization potentials of atoms calculated with a nonlocal exchange and a local correlation functional. International Journal of Quantum Chemistry, 1994, 52, 993-1010.	1.0	9
75	Density functional calculation of the photoabsorption spectrum of simple metal clusters: Beyond the local-density approximation and jellium model. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1994, 69, 1037-1044.	0.6	9
76	First principles calculation of the geometric and electronic structure of (Al2O3)n(Ox) clusters with n<15 and x=0, 1, 2. Thin Solid Films, 2003, 428, 206-210.	0.8	9
77	On the electric dipole moments of small sodium clusters from different theoretical approaches. Chemical Physics, 2012, 399, 252-257.	0.9	9
78	A non local density functional calculation of the diamagnetic susceptibilities and other electronic properties of noble gases and closed-shell ions. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1987, 6, 219-226.	1.0	8
79	A mass formula for the energy of metal clusters. International Journal of Quantum Chemistry, 1994, 52, 767-797.	1.0	8
80	Incipient manifestation of the shell structure of atoms within the WDA model for the exchange and kinetic energy density functionals. Chemical Physics, 1995, 196, 455-463.	0.9	8
81	Theoretical study of AlnV+ clusters and their interaction with Ar. Journal of Chemical Physics, 2013, 139, 214305.	1.2	8
82	Hydrogen Chemisorption on Doubly Vanadium Doped Aluminum Clusters. Zeitschrift Fur Physikalische Chemie, 2019, 233, 799-812.	1.4	8
83	Simple charge transfer model of X-ray scattering by ten-electron molecules. Molecular Physics, 1983, 50, 789-796.	0.8	7
84	Simple density functional theory of the electronegativity and other related properties of atoms and ions. , 1987, , 41-78.		7
85	Density functional theory of clusters of nontransition metals using simple models. Topics in Current Chemistry, 1996, , 119-171.	4.0	7
86	Is the vanadium(001) surface magnetic? Pseudopotential toward all-electron calculations. International Journal of Quantum Chemistry, 2003, 91, 230-233.	1.0	7
87	Theoretical study of CO adsorption on Au/alumina substrates. Physica Status Solidi (A) Applications and Materials Science, 2006, 203, 1277-1283.	0.8	7
88	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.	1.1	7
89	Density functional calculation of the electronegativity and other related properties of atoms and ions of the principal groups of the periodic table. Zeitschrift FÃ¼r Physik A, 1984, 319, 275-282.	1.4	6
90	Density functional theory of the chemical potential of atoms and its relation to electrostatic potentials and bonding distances. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1986, 1, 215-221.	1.0	6

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91	Comparison of the spherically averaged pseudopotential model with the stabilized jellium model. Journal of Physics B: Atomic, Molecular and Optical Physics, 1997, 30, 3583-3596.	0.6	6
92	Linear response to spin-dependent and spin-independent fields of alkali metal clusters. Journal of Physics Condensed Matter, 2000, 12, 4365-4380.	0.7	6
93	First principles study of CO adsorption-CO2 desorption mechanisms on oxidized doped-gold cationic clusters MAu n Oâ€‰m+ (M = Ti, Fe; n = 1,4-7; m = 1-2). International Journal of Quantum Chemistry, 2011, 111, 510-519.	1.0	6
94	On the chemical potential of atomic ions. Physics Letters, Section A: General, Atomic and Solid State Physics, 1984, 101, 20-22.	0.9	5
95	A mass formula for 4He clusters. Journal of Chemical Physics, 1991, 94, 7335-7341.	1.2	5
96	Photoabsorption cross sections of sodium clusters: electronic and geometrical effects. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1993, 26, 284-286.	1.0	5
97	Trends in the formation of aggregates and crystals from M@Si16 clusters: a study from first principle calculations. Journal of Mathematical Chemistry, 2010, 48, 109-117.	0.7	5
98	Structural, Vibrational, and Magnetic Properties of FeCoO_n^{0/+} (n = 1â€“6) Bimetallic Oxide Clusters. Journal of Physical Chemistry C, 2015, 119, 11200-11209.	1.5	5
99	Semiclassical variational study of size effects in neutral and charged jellium droplets. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1991, 19, 55-58.	1.0	4
100	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.	0.4	4
101	Antiferromagnetic versus ferromagnetic coupling in Fe/Cr(107) and Cr/Fe(107). Journal of Applied Physics, 1994, 76, 6989-6991.	1.1	4
102	Optical response of bimetallic and doped alkali clusters. Computational Materials Science, 1994, 2, 509-518.	1.4	4
103	DENSITY FUNCTIONAL STUDIES OF NOBLE METAL CLUSTERS. ADSORPTION OF O2 AND CO ON GOLD AND SILVER CLUSTERS. , 2006, , 407-432.		4
104	Study of oddâ€“even effects in physisorption and chemisorption of Ar, N₂, O₂ and NO on open shell Ag_{11â€“13}⁺ clusters by means of self-consistent van der Waals density functional calculations. Physical Chemistry Chemical Physics, 2019, 21, 25158-25174.	1.3	4
105	Relation between total energy, electronic potential at the nucleus, and chemical potential of positive ions. International Journal of Quantum Chemistry, 1984, 26, 145-149.	1.0	3
106	Magnetic properties of very thin V films adsorbed on Fe substrate. Journal of Magnetism and Magnetic Materials, 1993, 121, 177-179.	1.0	3
107	Hardness of metallic clusters. , 1993, , 229-257.		3
108	Density functional study of the stability and magnetic behaviour of AunTM+clusters (TM = Au, Sc, Ti, V,) Tj ETQq0 0 0 rgBT /Overlock 10	0.7	3

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109	Adsorption of H, H2, and H2O inside and outside of (M@Si16F)6 tubelike aggregates and wires (MÂ=ÂV, Ta). A first principles study. Materials Chemistry and Physics, 2013, 139, 247-255.	2.0	3
110	Multiple adsorption of molecular oxygen on small Au/Pd cationic clusters at finite temperature. A van der Waals density functional study. Journal of Chemical Physics, 2016, 144, 224308.	1.2	3
111	Relation between total energy, electronic potential at the nucleus and chemical potential. Application to the helium isoelectronic series in Hartree-Fock theory. Physics Letters, Section A: General, Atomic and Solid State Physics, 1983, 95, 89-91.	0.9	2
112	Nonlocal functionals for exchange and correlation in density functional theory: Application to atoms and to small atomic clusters. International Journal of Quantum Chemistry, 1995, 56, 499-508.	1.0	2
113	Slater sum for central field problems characterized by its s-wave component alone. Journal of Mathematical Physics, 1999, 40, 2671-2679.	0.5	2
114	Structure, fragmentation patterns, and electronic properties of small indium oxide clusters. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	2
115	Stepped Fe(100) and V/Fe(100) Magnetism. Materials Research Society Symposia Proceedings, 1991, 231, 323.	0.1	1
116	Magnetic properties of small 3-d transition metal clusters: Role of the sp-electrons and spd-hybridization. Scripta Materialia, 1993, 3, 359-363.	0.5	1
117	Calculation of the magnetic properties of FeN clusters embedded in 3d transition-metal matrices. Computational Materials Science, 1994, 2, 463-467.	1.4	1
118	Density functional study of photoabsorption in metallic clusters using an exchange-correlation potential with correct long-range behaviour. Journal of Physics Condensed Matter, 2002, 14, 5795-5812.	0.7	1
119	Density functional calculation of photoabsorption in metal clusters using an exchange-correlation potential with correct asymptotic behavior. International Journal of Quantum Chemistry, 2003, 91, 263-269.	1.0	1
120	Titanium embedded cage structure formation in AlnTi+ clusters and their interaction with Ar. Journal of Chemical Physics, 2014, 140, 174304.	1.2	1
121	A Combination of the Work Formalism for Exchange with an Optimized Correlation Energy Functional for Atoms. Journal De Physique II, 1995, 5, 1277-1287.	0.9	1
122	Density approximation to the average Hartree-Fock exchange potential for atoms. Journal of Chemical Sciences, 1994, 106, 91-102.	0.7	1
123	Nuclear-surface properties from a simple Thomas-Fermi calculation. Lettere Al Nuovo Cimento Rivista Internazionale Della SocietÃ Italiana Di Fisica, 1979, 26, 265-268.	0.4	0
124	Calculation of s-orbital hopping parameters for the tight-binding approach to chemisorption. Journal of Physics and Chemistry of Solids, 1986, 47, 751-758.	1.9	0
125	Self-consistent determination of surface and interface magnetism via the recursion method. Progress in Surface Science, 1990, 35, 51-54.	3.8	0
126	Optical response of bimetallic Li x Na8?x (0?x?8) and of doped Na8Zn clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1994, 31, 269-273.	1.0	0

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127	Semiclassical variational study of size effects in neutral and charged jellium droplets. , 1991, , 55-58.		0
128	Optical response of bimetallic Li x Na8â^'x (0â‰¦xâ‰¦8) and of doped Na8Zn clusters. , 1995, , 45-49.		0