Armando Beltran

List of Publications by Year
in descending order

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97 papers	4,097 citations	70961 41 h-index	123241 61 g-index
97 all docs	97 docs citations	97 times ranked	4755 citing authors

#	Article	IF	Citations
1	Crystal growth in colloidal tin oxide nanocrystals induced by coalescence at room temperature. Applied Physics Letters, 2003, 83, 1566-1568.	1.5	257
2	Density Functional Theory Study of the Brookite Surfaces and Phase Transitions between Natural Titania Polymorphs. Journal of Physical Chemistry B, 2006, 110, 23417-23423.	1.2	119
3	Topological analysis of electron density in depleted homopolar chemical bonds. Journal of Computational Chemistry, 1999, 20, 1517-1526.	1.5	115
4	Static simulation of bulk and selected surfaces of anatase TiO2. Surface Science, 2001, 490, 116-124.	0.8	115
5	Thermodynamic argument about SnO2 nanoribbon growth. Applied Physics Letters, 2003, 83, 635-637.	1.5	115
6	A Systematic Density Functional Theory Study of VxOy+ and VxOY (X = 2â^'4, Y = 2â^'10) Systems. Journal of Physical Chemistry A, 2001, 105, 9760-9775.	1.1	107
7	Room-temperature photoluminescence ofBaTiO3:â€ƒJoint experimental and theoretical study. Physical Review B, 2005, 71, .	1.1	103
8	Periodic study on the structural and electronic properties of bulk, oxidized and reduced SnO 2 (1 1 0) surfaces and the interaction with O 2. Surface Science, 2002, 511, 408-420.	0.8	100
9	Density functional theory calculation of the electronic structure ofBa0.5Sr0.5TiO3:Photoluminescent properties and structural disorder. Physical Review B, 2004, 69, .	1.1	98
10	Presence of excited electronic state in CaWO4 crystals provoked by a tetrahedral distortion: An experimental and theoretical investigation. Journal of Applied Physics, 2011, 110, .	1.1	84
11	A combined theoretical and experimental study of electronic structure and optical properties of Î²-ZnMoO4 microcrystals. Polyhedron, 2013, 54, 13-25.	1.0	83
12	Characterization of the High-Pressure Structures and Phase Transformations in SnO2. A Density Functional Theory Study. Journal of Physical Chemistry B, 2007, 111, 6479-6485.	1.2	82
13	Structure and Bonding of Chlorine Oxides and Peroxides:Â ClOx, ClOx-(x= 1â^'4), and Cl2Ox(x= 1â^'8). Journal of Physical Chemistry A, 1999, 103, 3078-3088.	1.1	74
14	A Joint Experimental and Theoretical Study on the Nanomorphology of CaWO₄ Crystals. Journal of Physical Chemistry C, 2011, 115, 20113-20119.	1.5	73
15	A theoretical study on the structure, energetics and bonding of VOx+ and VOx (x=1â€“4) systems. Chemical Physics Letters, 2001, 333, 493-503.	1.2	72
16	Topological Analysis of Multiple Metalâ^'Metal Bonds in Dimers of the M2(Formamidinate)4Type with M = Nb, Mo, Tc, Ru, Rh, and Pd. Journal of Physical Chemistry A, 2001, 105, 9460-9466.	1.1	71
17	Electronic and structural properties of SnxTi1â^'xO2 solid solutions: a periodic DFT study. Catalysis Today, 2003, 85, 145-152.	2.2	71
18	High-pressure study of the behavior of mineral barite by x-ray diffraction. Physical Review B, 2011, 84, .	1.1	71

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19	Structural and vibrational study of cubic Sb<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>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math> under high pressure. Physical Review B, 2012, 85, .	1.1	71
20	A theoretical analysis of adsorption and dissociation of CH3OH on the stoichiometric SnO2(110) surface. Surface Science, 1999, 430, 213-222.	0.8	70
21	Quantum-mechanical analysis of the equation of state of anataseTiO2. Physical Review B, 2001, 64, .	1.1	68
22	Theoretical Study on the Molecular Mechanism for the Reaction of VO2+ with C2H4. Journal of Physical Chemistry A, 2003, 107, 3107-3120.	1.1	68
23	Density Functional Theory Study on the Structural and Electronic Properties of Low Index Rutile Surfaces for TiO₂/SnO₂/TiO₂ and SnO₂/TiO₂/SnO₂ Composite Systems. Journal of Physical Chemistry A, 2008, 112, 8943-8952.	1.1	65
24	The hierarchy of localization basins: a tool for the understanding of chemical bonding exemplified by the analysis of the VO x and VO x + (x =1-4) systems. Theoretical Chemistry Accounts, 2001, 105, 299-308.	0.5	64
25	Structural and electronic properties of PbTiO3 slabs: a DFT periodic study. Surface Science, 2004, 552, 149-159.	0.8	62
26	DFT Study of the Reaction between VO2+ and C2H6. Organometallics, 2004, 23, 730-739.	1.1	61
27	Unveiling the Chemical and Morphological Features of Sbâ^'SnO₂ Nanocrystals by the Combined Use of High-Resolution Transmission Electron Microscopy and ab Initio Surface Energy Calculations. Journal of the American Chemical Society, 2009, 131, 14544-14548.	6.6	61
28	Origin of photoluminescence in SrTiO3: a combined experimental and theoretical study. Journal of Solid State Chemistry, 2004, 177, 3879-3885.	1.4	60
29	Isostructural Second-Order Phase Transition of Î²-Bi₂O₃ at High Pressures: An Experimental and Theoretical Study. Journal of Physical Chemistry C, 2014, 118, 23189-23201.	1.5	59
30	First-Principles Study of Pressure-Induced Phase Transitions and Electronic Properties of Ag₂MoO₄. Journal of Physical Chemistry C, 2014, 118, 3724-3732.	1.5	56
31	Lithium insertion and mobility in the TiO2-anatase/titanate structure: A periodic DFT study. Journal of Electroanalytical Chemistry, 2005, 581, 216-223.	1.9	52
32	Towards an insight on the photoluminescence of disordered CaWO4 from a joint experimental and theoretical analysis. Journal of Solid State Chemistry, 2005, 178, 1284-1291.	1.4	50
33	Contribution of structural order-disorder to the green photoluminescence ofPbWO4. Physical Review B, 2007, 75, .	1.1	48
34	A Combined Experimental and Theoretical Study on the Formation of Ag Filaments on Î²â€Ag₂MoO₄ Induced by Electron Irradiation. Particle and Particle Systems Characterization, 2015, 32, 646-651.	1.2	47
35	Experimental and Theoretical Study of Bi₂O₂Se Under Compression. Journal of Physical Chemistry C, 2018, 122, 8853-8867.	1.5	46
36	Insight into the Effects of Fe Addition on the Local Structure and Electronic Properties of SrTiO₃. Journal of Physical Chemistry C, 2014, 118, 4930-4940.	1.5	45

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37	Experimental and theoretical study of the ferroelectric and piezoelectric behavior of strontium-doped PZT. Journal of the European Ceramic Society, 2002, 22, 209-218.	2.8	44
38	Characterization of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiSiO</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:m and its pressure-induced phase transformations: Density functional theory study. Physical Review B, 2009, 80, .	1.1	44
39	Quantum-mechanical simulation ofMgAl2O4under high pressure. Physical Review B, 2002, 66, .	1.1	43
40	A theoretical analysis of the TiO2/Sn doped (110) surface properties. Surface Science, 2005, 580, 71-79.	0.8	42
41	Structural study of Î±-Bi₂O₃under pressure. Journal of Physics Condensed Matter, 2013, 25, 475402.	0.7	42
42	Experimental and theoretical investigation of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>ThGeO</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml: high pressure. Physical Review B, 2009, 80, .	1.1	40
43	CaSO₄ and Its Pressure-Induced Phase Transitions. A Density Functional Theory Study. Inorganic Chemistry, 2012, 51, 1751-1759.	1.9	38
44	Combined Experimental and Theoretical Study to Understand the Photoluminescence of Sr1-xTiO3-x. Journal of Physical Chemistry B, 2004, 108, 9221-9227.	1.2	37
45	Theoretical study of the structure and stability of NbxOy and NbxOy+ (x=1â€“3; y=2â€“5,â€˜7,â€˜8) clusters. Chemical Physics Letters, 1998, 287, 620-626.	1.2	36
46	Origin of the low compressibility in hard nitride spinels. Physical Review B, 2003, 68, .	1.1	36
47	Theoretical study of ZnO (1010) and Cu/ZnO (1010) surfaces. Chemical Physics Letters, 2001, 338, 224-230.	1.2	35
48	A Theoretical Study on the Pressure-Induced Phase Transitions in the Inverse Spinel Structure Zn₂SnO₄. Journal of Physical Chemistry C, 2011, 115, 7740-7746.	1.5	35
49	Anomalous oriented attachment growth behavior on SnO2 nanocrystals. Chemical Communications, 2011, 47, 3117.	2.2	35
50	Effect of Pressure-Assisted Heat Treatment on Photoluminescence Emission of Î±-Bi₂O₃ Needles. Inorganic Chemistry, 2015, 54, 10184-10191.	1.9	33
51	Mechanistic Insights into the Reaction between VO2+ and Propene Based on a DFT Study. Organometallics, 2006, 25, 1643-1653.	1.1	28
52	Enhancement of optical absorption by modulation of the oxygen flow of TiO2 films deposited by reactive sputtering. Journal of Applied Physics, 2012, 111, .	1.1	28
53	Structural and Electronic Effects of Incorporating Mn in TiO₂ Films Grown by Sputtering: Anatase versus Rutile. Journal of Physical Chemistry C, 2012, 116, 8753-8762.	1.5	28
54	An ab initio perturbed ion study of structural properties of TiO2, SnO2 and GeO2 rutile lattices. Chemical Physics, 1996, 212, 381-391.	0.9	27

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55	A Theoretical Study on the Gas Phase Reactions of the Anions NbO3-, NbO5-, and NbO2(OH)2- with H2O and O2. Journal of Physical Chemistry A, 2004, 108, 10850-10860.	1.1	26
56	Electronic structure and magnetic properties of FeWO4 nanocrystals synthesized by the microwave-hydrothermal method. Materials Characterization, 2012, 73, 124-129.	1.9	26
57	DFT study of the water-assisted tautomerization process between hydrated oxide, MO(H2O)+, and dihydroxide, M(OH)2+, cations (M=V, Nb and Ta). Chemical Physics Letters, 2004, 384, 56-62.	1.2	25
58	Intercalation processes and diffusion paths of lithium ions in spinel-type structured<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Li</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>+</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="normal">Ti</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math>: Density functional theory. Physical Review B, 2008, 77, .	1.1	25
59	Am1 and pm3 transition structure for the hydride transfer. A model of reaction catalyzed by dihydrofolate reductase. Computational and Theoretical Chemistry, 1995, 330, 411-416.	1.5	24
60	Ab initio cluster-in-the-lattice description of vanadium-doped zircon: analysis of the impurity centers in vanadium(4+)-doped zircon (ZrSiO4). The Journal of Physical Chemistry, 1993, 97, 2555-2559.	2.9	23
61	Synthesis, optical and ferroelectric properties of PZT thin films: experimental and theoretical investigation. Journal of Materials Chemistry, 2012, 22, 6587.	6.7	22
62	First-Principles Study on Polymorphs of AgVO₃: Assessing to Structural Stabilities and Pressure-Induced Transitions. Journal of Physical Chemistry C, 2017, 121, 27624-27642.	1.5	22
63	An atom-in-molecules and electron-localization-function study of the interaction between O 2 and V x O y + /V x O y (x = 1, 2, y = 1-5) clusters. Theoretical Chemistry Accounts, 2002, 108, 12-20.	0.5	21
64	Pressure-induced phase transitions in AgClO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>. Physical Review B, 2011, 84, .	1.1	21
65	Pressure effects on the vibrational properties ofÎ±-Bi₂O₃: an experimental and theoretical study. Journal of Physics Condensed Matter, 2014, 26, 225401.	0.7	21
66	Theoretical and experimental study of the relation between photoluminescence and structural disorder in barium and strontium titanate thin films. Journal of the European Ceramic Society, 2005, 25, 2337-2340.	2.8	19
67	Dopant Segregation Analysis on Sb:SnO₂ Nanocrystals. Chemistry - A European Journal, 2011, 17, 11515-11519.	1.7	19
68	Structural and Electronic Properties of Lithiated SnO₂. A Periodic DFT Study. Journal of Physical Chemistry C, 2012, 116, 16127-16137.	1.5	19
69	Experimental and theoretical study on the piezoelectric behavior of barium doped PZT. Journal of Materials Science, 1999, 34, 3659-3667.	1.7	17
70	Piezoelectric behaviour of PZT doped with calcium: a combined experimental and theoretical study. Journal of Materials Science, 1997, 32, 2381-2386.	1.7	16
71	An ab initio study of oxygen vacancies and doping process of Nb and Cr atoms on TiO2 (110) surface models. International Journal of Quantum Chemistry, 1997, 65, 625-631.	1.0	16
72	A theoretical analysis on electronic structure of the (110) surface of TiO2â€“SnO2 mixed oxide. Computational and Theoretical Chemistry, 2003, 629, 307-314.	1.5	16

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73	Pb1â^'xCaxTiO3solid solution (x=0.0, 0.25, 0.50, and 0.75): A theoretical and experimental approach. Physical Review B, 2007, 75, .	1.1	16
74	Quantum mechanical modeling of excited electronic states and their relationship to cathodoluminescence of BaZrO3. Journal of Applied Physics, 2013, 114, .	1.1	16
75	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î²</mml:mi><mml:mo>â^'</mml:mo><mml:mi mathvariant="normal">B</mml:mi><mml:msub><mml:mi mathvariant="normal">i</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>under compression: Optical and elastic properties and electron density topology analysis. Physical Review B,	1.1	16
76	Polymorphs of ZnV₂O₆ under Pressure: A First-Principle Investigation. Journal of Physical Chemistry C, 2019, 123, 3239-3253.	1.5	16
77	Experimental and Theoretical Study of SbPO4 under Compression. Inorganic Chemistry, 2020, 59, 287-307.	1.9	14
78	Composition Dependence of the Energy Barrier for Lithium Diffusion in Amorphous WO[sub 3]. Electrochemical and Solid-State Letters, 2005, 8, J21.	2.2	13
79	Theoretical Third-Order Hyperpolarizability of Paratellurite from the Finite Field Perturbation Method. Journal of Physical Chemistry B, 2008, 112, 10777-10781.	1.2	13
80	Pseudopotential Periodic Hartree-Fock study of K8In11 and Rb8In11 Systems. The Journal of Physical Chemistry, 1995, 99, 12483-12487.	2.9	10
81	Room temperature photoluminescence of the Li2ZnTi3O8spinel: Experimental and theoretical study. International Journal of Quantum Chemistry, 2005, 103, 580-587.	1.0	10
82	Garnet Crystal Structures. An ab Initio Perturbed Ion Study. The Journal of Physical Chemistry, 1995, 99, 6493-6501.	2.9	9
83	Prediction of dopant atom distribution on nanocrystals using thermodynamic arguments. Physical Chemistry Chemical Physics, 2014, 16, 1089-1094.	1.3	9
84	Local Relaxation Effects in the Crystal Structure of Vanadium-Doped Zircon. An ab Initio Perturbed Ion Calculation. The Journal of Physical Chemistry, 1994, 98, 7741-7744.	2.9	8
85	Bonding and compressibility in molecular and polymeric phases of solid CO2. Journal of Physics Condensed Matter, 2004, 16, S1263-S1270.	0.7	8
86	An ab initio perturbed ion study of bulk ceria. Chemical Physics Letters, 1994, 221, 249-254.	1.2	7
87	Periodic Hartree-Fock calculation of the A1g (Tz) and Eg (Tx, Ty) phonon modes in ice VIII. Journal of Molecular Structure, 1997, 436-437, 443-449.	1.8	5
88	Propriedades eletrÃ´nicas e estruturais do PbTiO3: teoria do funcional de densidade aplicada a modelos periÃ³dicos. Quimica Nova, 2005, 28, 10-18.	0.3	5
89	DFT study on the water-assisted mechanism for the reaction between VO+ and NH3 to yield VNH+ and H2O. Chemical Physics Letters, 2006, 427, 265-270.	1.2	5
90	Bonding changes across the Î±-cristobaliteâ†'stishovite transition path in silica. High Pressure Research, 2009, 29, 93-96.	0.4	5

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91	An Ab initio perturbed ion study of pyrope garnet structure. Journal of Physics and Chemistry of Solids, 1995, 56, 901-906.	1.9	4
92	Simulation of ionic crystals: calculation of Madelung potentials for stabilized zirconia. Journal of Materials Science, 1995, 30, 4852-4856.	1.7	3
93	An ab Initio Perturbed Ion Study of the BaLiF3 and BaLiH3 Inverted Perovskite Structures. The Journal of Physical Chemistry, 1995, 99, 8082-8090.	2.9	3
94	Thermodynamic and electronic study of Ga1â^'xMnxN films. A theoretical study. Surface Science, 2011, 605, 1431-1437.	0.8	3
95	Fotoluminiscencia del PbTiO₃ en estado amorfo analizada por mÃ©todos ab-initio periÃ³dicos. Boletin De La Sociedad Espanola De Ceramica Y Vidrio, 2004, 43, 644-648.	0.9	3
96	Theoretical study of lattice stability and selective doping effects of V4+ and Tb4+ in the ZrGeO4 lattice. Chemical Physics Letters, 1995, 236, 521-531.	1.2	2
97	Ab initio perturbed ion calculations on Ni2+Â·KZnF3 and Ni2+ Â·KMgF3. A structural study. Computational and Theoretical Chemistry, 1995, 330, 319-323.	1.5	2