Armando Beltran

List of Publications by Citations

96 papers	3,660 citations	38 h-index	56 g-index
97 ext. papers	3,852 ext. citations	3.3 avg, IF	4.8 L-index

#	Paper	IF	Citations
96	Crystal growth in colloidal tin oxide nanocrystals induced by coalescence at room temperature. *Applied Physics Letters*, **2003**, 83, 1566-1568	3.4	237
95	Topological analysis of electron density in depleted homopolar chemical bonds. *Journal of Computational Chemistry*, **1999**, 20, 1517-1526	3.5	107
94	Static simulation of bulk and selected surfaces of anatase TiO2. *Surface Science*, **2001**, 490, 116-124	1.8	106
93	Thermodynamic argument about SnO2 nanoribbon growth. *Applied Physics Letters*, **2003**, 83, 635-637	3.4	105
92	Density functional theory study of the brookite surfaces and phase transitions between natural titania polymorphs. *Journal of Physical Chemistry B*, **2006**, 110, 23417-23	3.4	103
91	A Systematic Density Functional Theory Study of VxOy+ and VxOY (X = 2□, Y = 2□0) Systems. *Journal of Physical Chemistry A*, **2001**, 105, 9760-9775	2.8	102
90	Density functional theory calculation of the electronic structure of Ba0.5Sr0.5TiO3: Photoluminescent properties and structural disorder. *Physical Review B*, **2004**, 69,	3.3	94
89	Room-temperature photoluminescence of BaTiO3: Joint experimental and theoretical study. *Physical Review B*, **2005**, 71,	3.3	93
88	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	1.8	92
87	Presence of excited electronic state in CaWO4 crystals provoked by a tetrahedral distortion: An experimental and theoretical investigation. *Journal of Applied Physics*, **2011**, 110, 043501	2.5	74
86	Structure and Bonding of Chlorine Oxides and Peroxides:´ ClOx, ClOx-(x= 1□), and Cl2Ox(x= 1□). *Journal of Physical Chemistry A*, **1999**, 103, 3078-3088	2.8	69
85	Theoretical Study on the Molecular Mechanism for the Reaction of VO2+ with C2H4. *Journal of Physical Chemistry A*, **2003**, 107, 3107-3120	2.8	68
84	A Joint Experimental and Theoretical Study on the Nanomorphology of CaWO4 Crystals. *Journal of Physical Chemistry C*, **2011**, 115, 20113-20119	3.8	66
83	Electronic and structural properties of SnxTi1□O2 solid solutions: a periodic DFT study. *Catalysis Today*, **2003**, 85, 145-152	5.3	66
82	A theoretical study on the structure, energetics and bonding of VOx+ and VOx (x=1□) systems. *Chemical Physics Letters*, **2001**, 333, 493-503	2.5	66
81	A combined theoretical and experimental study of electronic structure and optical properties of □ZnMoO4 microcrystals. *Polyhedron*, **2013**, 54, 13-25	2.7	65
80	Characterization of the high-pressure structures and phase transformations in SnO2. A density functional theory study. *Journal of Physical Chemistry B*, **2007**, 111, 6479-85	3.4	65

79	A theoretical analysis of adsorption and dissociation of CH3OH on the stoichiometric SnO2(110) surface. *Surface Science*, **1999**, 430, 213-222	1.8	65
78	The hierarchy of localization basins: a tool for the understanding of chemical bonding exemplified by the analysis of the VOx and VOx+ (x=1,2) systems. *Theoretical Chemistry Accounts*, **2001**, 105, 299-308	1.9	63
77	Quantum-mechanical analysis of the equation of state of anatase TiO2. *Physical Review B*, **2001**, 64,	3.3	63
76	Topological Analysis of Multiple Metal−Metal Bonds in Dimers of the M2(Formamidinate)4 Type with M = Nb, Mo, Tc, Ru, Rh, and Pd. *Journal of Physical Chemistry A*, **2001**, 105, 9460-9466	2.8	62
75	DFT Study of the Reaction between VO2+ and C2H6. *Organometallics*, **2004**, 23, 730-739	3.8	61
74	High-pressure study of the behavior of mineral barite by x-ray diffraction. *Physical Review B*, **2011**, 84,	3.3	59
73	Structural and vibrational study of cubic Sb2O3 under high pressure. *Physical Review B*, **2012**, 85,	3.3	57
72	Origin of photoluminescence in SrTiO3: a combined experimental and theoretical study. *Journal of Solid State Chemistry*, **2004**, 177, 3879-3885	3.3	57
71	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, 8943-52	2.8	55
70	Unveiling the chemical and morphological features of Sb-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, 14544-8	16.4	52
69	Structural and electronic properties of PbTiO3 slabs: a DFT periodic study. *Surface Science*, **2004**, 552, 149-159	1.8	52
68	Isostructural Second-Order Phase Transition of β-Bi2O3 at High Pressures: An Experimental and Theoretical Study. *Journal of Physical Chemistry C*, **2014**, 118, 23189-23201	3.8	50
67	Lithium insertion and mobility in the TiO2-anatase/titanate structure: A periodic DFT study. *Journal of Electroanalytical Chemistry*, **2005**, 581, 216-223	4.1	47
66	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	3.3	46
65	Contribution of structural order-disorder to the green photoluminescence of PbWO4. *Physical Review B*, **2007**, 75,	3.3	44
64	First-Principles Study of Pressure-Induced Phase Transitions and Electronic Properties of Ag2MoO4. *Journal of Physical Chemistry C*, **2014**, 118, 3724-3732	3.8	42
63	A Combined Experimental and Theoretical Study on the Formation of Ag Filaments on β-Ag2MoO4 Induced by Electron Irradiation. *Particle and Particle Systems Characterization*, **2015**, 32, 646-651	3.1	41
62	Experimental and theoretical study of the ferroelectric and piezoelectric behavior of strontium-doped PZT. *Journal of the European Ceramic Society*, **2002**, 22, 209-218	6	41

61	A theoretical analysis of the TiO2/Sn doped (1 1 0) surface properties. *Surface Science*, **2005**, 580, 71-79	1.8	41
60	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	3.8	40
59	Characterization of the TiSiO4 structure and its pressure-induced phase transformations: Density functional theory study. *Physical Review B*, **2009**, 80,	3.3	40
58	Quantum-mechanical simulation of MgAl2O4 under high pressure. *Physical Review B*, **2002**, 66,	3.3	37
57	CaSO4 and its pressure-induced phase transitions. A density functional theory study. *Inorganic Chemistry*, **2012**, 51, 1751-9	5.1	36
56	Combined Experimental and Theoretical Study to Understand the Photoluminescence of Sr1-xTiO3-x. *Journal of Physical Chemistry B*, **2004**, 108, 9221-9227	3.4	36
55	Experimental and theoretical investigation of ThGeO4 at high pressure. *Physical Review B*, **2009**, 80,	3.3	35
54	Theoretical study of the structure and stability of NbxOy and NbxOy+ (x=1□; y=2□, 7, 8) clusters. *Chemical Physics Letters*, **1998**, 287, 620-626	2.5	35
53	Origin of the low compressibility in hard nitride spinels. *Physical Review B*, **2003**, 68,	3.3	34
52	Theoretical study of ZnO (1010) and Cu/ZnO (1010) surfaces. *Chemical Physics Letters*, **2001**, 338, 224-230	2.5	34
51	Experimental and Theoretical Study of Bi2O2Se Under Compression. *Journal of Physical Chemistry C* , **2018**, 122, 8853-8867	3.8	32
50	Anomalous oriented attachment growth behavior on SnO2 nanocrystals. *Chemical Communications*, **2011**, 47, 3117-9	5.8	32
49	A Theoretical Study on the Pressure-Induced Phase Transitions in the Inverse Spinel Structure Zn2SnO4. *Journal of Physical Chemistry C*, **2011**, 115, 7740-7746	3.8	28
48	Mechanistic Insights into the Reaction between VO2+ and Propene Based on a DFT Study. *Organometallics*, **2006**, 25, 1643-1653	3.8	28
47	Structural study of □Bi2O3 under pressure. *Journal of Physics Condensed Matter*, **2013**, 25, 475402	1.8	27
46	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	3.8	27
45	Enhancement of optical absorption by modulation of the oxygen flow of TiO2 films deposited by reactive sputtering. *Journal of Applied Physics*, **2012**, 111, 113513	2.5	25
44	Effect of Pressure-Assisted Heat Treatment on Photoluminescence Emission of □Bi2O3 Needles. *Inorganic Chemistry*, **2015**, 54, 10184-91	5.1	24

43	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	2.5	24
42	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	2.8	24
41	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		24
40	An ab initio perturbed ion study of structural properties of TiO2, SnO2 and GeO2 rutile lattices. *Chemical Physics*, **1996**, 212, 381-391	2.3	24
39	Intercalation processes and diffusion paths of lithium ions in spinel-type structured Li1+xTi2O4: Density functional theory study. *Physical Review B*, **2008**, 77,	3.3	22
38	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		21
37	Pressure-induced phase transitions in AgClO4. *Physical Review B*, **2011**, 84,	3.3	20
36	First-Principles Study on Polymorphs of AgVO3: Assessing to Structural Stabilities and Pressure-Induced Transitions. *Journal of Physical Chemistry C*, **2017**, 121, 27624-27642	3.8	19
35	Electronic structure and magnetic properties of FeWO4 nanocrystals synthesized by the microwave-hydrothermal method. *Materials Characterization*, **2012**, 73, 124-129	3.9	19
34	An atom-in-molecules and electron-localization-function study of the interaction between O2 and VxOy+/VxOy (x = 1, 2, y = 1□) clusters. *Theoretical Chemistry Accounts*, **2002**, 108, 12-20	1.9	19
33	Synthesis, optical and ferroelectric properties of PZT thin films: experimental and theoretical investigation. *Journal of Materials Chemistry*, **2012**, 22, 6587		18
32	Dopant segregation analysis on Sb:SnO2 nanocrystals. *Chemistry - A European Journal*, **2011**, 17, 11515-9	4.8	18
31	Pressure effects on the vibrational properties of □Bi(2)O(3): an experimental and theoretical study. *Journal of Physics Condensed Matter*, **2014**, 26, 225401	1.8	17
30	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	6	17
29	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	2.1	16
28	A theoretical analysis on electronic structure of the (110) surface of TiO2□SnO2 mixed oxide. *Computational and Theoretical Chemistry*, **2003**, 629, 307-314		16
27	Experimental and theoretical study on the piezoelectric behavior of barium doped PZT. *Journal of Materials Science*, **1999**, 34, 3659-3667	4.3	16
26	**B**i2O3 under compression: Optical and elastic properties and electron density topology analysis. *Physical Review B*, **2016**, 93,	3.3	15

25	Quantum mechanical modeling of excited electronic states and their relationship to cathodoluminescence of BaZrO3. *Journal of Applied Physics*, **2013**, 114, 043714	2.5	15
24	Structural and Electronic Properties of Lithiated SnO2. A Periodic DFT Study. *Journal of Physical Chemistry C*, **2012**, 116, 16127-16137	3.8	14
23	Piezoelectric behaviour of PZT doped with calcium: a combined experimental and theoretical study. *Journal of Materials Science*, **1997**, 32, 2381-2386	4.3	14
22	Theoretical third-order hyperpolarizability of paratellurite from the finite field perturbation method. *Journal of Physical Chemistry B*, **2008**, 112, 10777-81	3.4	12
21	Pb1⊠CaxTiO3 solid solution (x=0.0, 0.25, 0.50, and 0.75): A theoretical and experimental approach. *Physical Review B*, **2007**, 75,	3.3	12
20	Polymorphs of ZnV2O6 under Pressure: A First-Principle Investigation. *Journal of Physical Chemistry C*, **2019**, 123, 3239-3253	3.8	11
19	Pseudopotential Periodic Hartree-Fock study of K8In11 and Rb8In11 Systems. *The Journal of Physical Chemistry*, **1995**, 99, 12483-12487		10
18	Room temperature photoluminescence of the Li2ZnTi3O8 spinel: Experimental and theoretical study. *International Journal of Quantum Chemistry*, **2005**, 103, 580-587	2.1	9
17	Composition Dependence of the Energy Barrier for Lithium Diffusion in Amorphous WO[sub 3]. *Electrochemical and Solid-State Letters*, **2005**, 8, J21		9
16	Experimental and Theoretical Study of SbPO under Compression. *Inorganic Chemistry*, **2020**, 59, 287-307	5.1	9
15	Prediction of dopant atom distribution on nanocrystals using thermodynamic arguments. *Physical Chemistry Chemical Physics*, **2014**, 16, 1089-94	3.6	8
14	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		8
13	Bonding and compressibility in molecular and polymeric phases of solid CO2. *Journal of Physics Condensed Matter*, **2004**, 16, S1263-S1270	1.8	7
12	Garnet Crystal Structures. An ab Initio Perturbed Ion Study. *The Journal of Physical Chemistry*, **1995**, 99, 6493-6501		7
11	An ab initio perturbed ion study of bulk ceria. *Chemical Physics Letters*, **1994**, 221, 249-254	2.5	6
10	Bonding changes across the ⊟ristobalite-stishovite transition path in silica. *High Pressure Research*, **2009**, 29, 93-96	1.6	5
9	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	3.4	5
8	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	2.5	5

7	Propriedades eletrônicas e estruturais do PbTiO3: teoria do funcional de densidade aplicada a modelos periódicos. *Quimica Nova*, **2005**, 28, 10-18	1.6	4
6	An Ab initio perturbed ion study of pyrope garnet structure. *Journal of Physics and Chemistry of Solids*, **1995**, 56, 901-906	3.9	4
5	Thermodynamic and electronic study of Ga1−xMnxN films. A theoretical study. *Surface Science*, **2011**, 605, 1431-1437	1.8	3
4	An ab Initio Perturbed Ion Study of the BaLiF3 and BaLiH3 Inverted Perovskite Structures. *The Journal of Physical Chemistry*, **1995**, 99, 8082-8090		3
3	Theoretical study of lattice stability and selective doping effects of V4+ and Tb4+ in the ZrGeO4 lattice. *Chemical Physics Letters*, **1995**, 236, 521-531	2.5	2
2	Simulation of ionic crystals: calculation of Madelung potentials for stabilized zirconia. *Journal of Materials Science*, **1995**, 30, 4852-4856	4.3	1
1	Ab initio perturbed ion calculations on Ni2+ KZnF3 and Ni2+ KMgF3. A structural study. *Computational and Theoretical Chemistry*, **1995**, 330, 319-323		1