Adilmo Lima

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Electronic and optical properties of multifunctional R3c AFeO3 (A = Sc or In) compounds: Insights into their potential for photovoltaic applications. Journal of Physics and Chemistry of Solids, 2022, 160, 110346.	4.0	4
2	Electronic, optical, and photocatalytic properties of the wolframite InNbO4 and InTaO4 compounds. Optical Materials, 2022, 123, 111781.	3.6	1
3	Magnetic and electronic properties of the RECu4Al8 (RE = Tb, Dy, Ho, and Er) intermetallic compounds. Intermetallics, 2022, 143, 107474.	3.9	1
4	Exchange interactions in hexagonal YMnO3 and LuMnO3 multiferroic compounds. Journal of Solid State Chemistry, 2021, 299, 122175.	2.9	2
5	Ab initio study of the phonon and thermodynamic properties of the scheelite MWO4 (M = Ba, Sr or Ca) compounds. Solid State Communications, 2021, 333, 114290.	1.9	2
6	Non-collinear spin DFT study of the ground state magnetic structure, optical and electronic properties of the hexagonal LuFeO3 multiferroic. Journal of Alloys and Compounds, 2020, 813, 152227.	5.5	6
7	The structural, magnetic and electronic properties of the ground state of the hexagonal LuMnO ₃ multiferroic. Physica Scripta, 2020, 95, 085801.	2.5	5
8	Structural, electronic and optical characterization of substitutional Ag defect in Li2B4O7 scintillator. Journal of Physics and Chemistry of Solids, 2020, 146, 109615.	4.0	4
9	Optical properties, energy band gap and the charge carriers' effective masses of the R3c BiFeO3 magnetoelectric compound. Journal of Physics and Chemistry of Solids, 2020, 144, 109484.	4.0	22
10	Theoretical study of electronic and optical properties of the scheelite MWO4 (M = Ca, Sr or Ba) compounds by applying the modified Becke-Johnson exchange-correlation potential. Optical Materials, 2019, 92, 187-194.	3.6	17
11	Theoretical study of structural, electronic and magnetic properties of the spinel Co3O4 under the pressure from 0 to 30†GPa. Journal of Magnetism and Magnetic Materials, 2019, 484, 21-30.	2.3	10
12	Comparative study of magnetic and electronic properties of roomâ€ŧemperature polar magnets ScFeO ₃ and InFeO ₃ . International Journal of Quantum Chemistry, 2019, 119, e25846.	2.0	2
13	Atomistic simulation study of the ferroelectric and paraelectric phases of the hexagonal RMnO3 (R =) Tj ETQq1 1	0.78431	4 rgBT /Over
14	First-principles study of structural, electronic, energetic and optical properties of substitutional Cu defect in Li2B4O7 scintillator. Journal of Alloys and Compounds, 2018, 735, 756-764.	5.5	8
15	Optical absorption spectrum and electronic structure of multiferroic hexagonal YMnO 3 compound. Optical Materials, 2017, 64, 406-412.	3.6	9
16	Antisite defect as rule for photorefractive, photochromic and photocatalytic properties of Bi 12 MO 20 (MÂ=ÂGe, Si, Ti) sillenite crystals. Journal of Alloys and Compounds, 2017, 720, 187-195.	5.5	30
17	New insights into the electronic and optical properties of the Bi4M3O12 (MÂ= Si or Ge) scintillators. Optical Materials, 2017, 73, 642-646.	3.6	6
18	Ground-state magnetic structure of hexagonal YMnO3 compound: A non-collinear spin density functional theory study. Journal of Magnetism and Magnetic Materials, 2016, 416, 236-240.	2.3	11

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19	Electronic structure and optical properties of magnesium tetraborate: An ab initio study. Computational Materials Science, 2016, 124, 1-7.	3.0	21
20	Atomistic simulation of trivalent ions doped in the hexagonal LuMnO3 ferroelectric phase. Journal of Alloys and Compounds, 2016, 689, 977-982.	5.5	8
21	Density functional theory study on the magnetic properties of Co3O4 with normal spinel structure. Journal of Physics and Chemistry of Solids, 2016, 91, 86-89.	4.0	11
22	Analysis of the Mn–O and Y–O bonds in paraelectric and ferroelectric phase of magnetoelectric YMnO 3 from the first principles calculations. Journal of Alloys and Compounds, 2015, 649, 285-290.	5.5	12
23	Structural, bonding, and electronic properties of the hexagonal ferroelectric and paraelectric phases of LuMnO3 compound: A density functional theory study. Journal of Chemical Physics, 2015, 142, 074703.	3.0	14
24	Interpretation of the optical absorption spectrum of Co3O4 with normal spinel structure from first principles calculations. Journal of Physics and Chemistry of Solids, 2014, 75, 148-152.	4.0	20
25	Electronic structure and optical properties of lithium tetraborate detector calculated using semi-local exchange correlation potential. Computational Materials Science, 2014, 95, 271-275.	3.0	13
26	Analysis of Orbital Hybridization in the Magnetoelectric \${hbox{YMnO}}_{3}\$ Crystal From First Principles Calculations. IEEE Transactions on Magnetics, 2013, 49, 4687-4690.	2.1	4
27	First-principles study of the Bi _M O ₄ antisite defect in the Bi ₁₂ MO ₂₀ (M=Si, Ge, Ti) sillenite compounds. Journal of Physics Condensed Matter, 2013, 25, 495505.	1.8	9
28	An <i>ab-initio</i> study of electronic and optical properties of corundum Al2O3 doped with Sc, Y, Zr, and Nb. Journal of Applied Physics, 2012, 112, .	2.5	27
29	Structural, electronic, optical, and magneto-optical properties of Bi12MO20 (M = Ti, Ge, Si) sillenite crystals from first principles calculations. Journal of Applied Physics, 2011, 110, .	2.5	43
30	First principles study of electronic and optical properties of the chromium doped BGO crystal. Journal of Physics: Conference Series, 2010, 249, 012035.	0.4	0
31	Thermoluminescent properties studies of spodumene lilac sample to dosimetric applications. Journal of Physics: Conference Series, 2010, 249, 012013.	0.4	5
32	Structural, electronic, and optical aspects of Cr doping of the Bi4Ge3O12: An ab initio study. Journal of Applied Physics, 2010, 108, 083713.	2.5	1
33	Effects of transition metal impurities in alpha alumina: a theoretical study. Journal of Physics: Conference Series, 2010, 249, 012036.	0.4	1
34	Ab initio study of structural, electronic and optical properties of the Bi12TiO20 sillenite crystal. Computational Materials Science, 2010, 49, 321-325.	3.0	13
35	Electronic structure and optical absorption of the Bi4Ge3O12 and the Bi4Si3O12 scintillators in ultraviolet region: An <i>ab initio</i> study. Journal of Applied Physics, 2009, 106, .	2.5	27
36	Theoretical analysis of optical characteristics of the alpha spodumene in ultraviolet region. Optical Materials, 2009, 31, 1478-1482.	3.6	9

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37	Optical properties of alpha spodumene: Orientation of its principal optical axes. Journal of Physics: Conference Series, 2009, 167, 012066.	0.4	1
38	Electronic and optical properties of spodumene gemstone: A theoretical study. Optical Materials, 2008, 30, 1048-1051.	3.6	12
39	Thermoluminescent Mechanism in Lilac Spodumene. Acta Physica Polonica A, 2007, 112, 1001-1006.	0.5	12