

Marisa Carvalho Oliveira

List of Publications by Year in descending order

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papers

786
citations

430442

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525886

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37
all docs

37
docs citations

37
times ranked

630
citing authors

#	ARTICLE	IF	CITATIONS
1	Connecting the surface structure, morphology and photocatalytic activity of Ag ₂ O: An in depth and unified theoretical investigation. Applied Surface Science, 2020, 509, 145321.	3.1	51
2	Connecting theory with experiment to understand the photocatalytic activity of CuO@ZnO heterostructure. Ceramics International, 2020, 46, 9446-9454.	2.3	50
3	Role of Surfaces in the Magnetic and Ozone Gas-Sensing Properties of ZnFe ₂ O ₄ Nanoparticles: Theoretical and Experimental Insights. ACS Applied Materials & Interfaces, 2021, 13, 4605-4617.	4.0	49
4	Structural, electronic, vibrational and magnetic properties of Zn ²⁺ substituted MnCr ₂ O ₄ nanoparticles. Journal of Magnetism and Magnetic Materials, 2020, 502, 166595.	1.0	48
5	A theoretical investigation of the structural and electronic properties of orthorhombic CaZrO ₃ . Ceramics International, 2015, 41, 3069-3074.	2.3	45
6	Synthesis and morphological transformation of BaWO ₄ crystals: Experimental and theoretical insights. Ceramics International, 2016, 42, 10913-10921.	2.3	45
7	Understanding the White-Emitting CaMoO ₄ Co-Doped Eu ³⁺ , Tb ³⁺ , and Tm ³⁺ Phosphor through Experiment and Computation. Journal of Physical Chemistry C, 2019, 123, 18536-18550.	1.5	45
8	Experimental and theoretical study to explain the morphology of CaMoO ₄ crystals. Journal of Physics and Chemistry of Solids, 2018, 114, 141-152.	1.9	42
9	Structure, morphology and photoluminescence emissions of ZnMoO ₄ : RE ³⁺ =Tb ³⁺ - Tm ³⁺ - X Eu ³⁺ (x= 1, 0.784314) Compounds, 2018, 750, 55-70.	2.8	34
10	Structural, electronic and magnetic properties of Sc ³⁺ doped CoCr ₂ O ₄ nanoparticles. New Journal of Chemistry, 2020, 44, 14246-14255.	1.4	31
11	Towards shape-oriented Bi-doped CoCr ₂ O ₄ nanoparticles from theoretical and experimental perspectives: structural, morphological, optical, electrical and magnetic properties. Journal of Materials Chemistry C, 2021, 9, 6452-6469.	2.7	29
12	Recent progress and approaches on the synthesis of Mn-doped zinc oxide nanoparticles: a theoretical and experimental investigation on the photocatalytic performance. New Journal of Chemistry, 2020, 44, 8805-8812.	1.4	28
13	On the morphology of BaMoO ₄ crystals: A theoretical and experimental approach. Crystal Research and Technology, 2016, 51, 634-644.	0.6	24
14	Geometry, electronic structure, morphology, and photoluminescence emissions of BaW _{1-x} Mo _x O ₄ (x=0, 0.25, 0.50, 0.75, and 1) solid solutions: Theory and experiment in concert. Applied Surface Science, 2019, 463, 907-917.	3.1	24
15	Temperature dependence on phase evolution in the BaTiO ₃ polytypes studied using ab initio calculations. International Journal of Quantum Chemistry, 2020, 120, e26054.	1.0	23
16	Experimental and theoretical study of the energetic, morphological, and photoluminescence properties of CaZrO ₃ :Eu ³⁺ . CrystEngComm, 2018, 20, 5519-5530.	1.3	22
17	Disclosing the Structural, Electronic, Magnetic, and Morphological Properties of CuMnO ₂ : A Unified Experimental and Theoretical Approach. Journal of Physical Chemistry C, 2020, 124, 5378-5388.	1.5	22
18	Computational Chemistry Meets Experiments for Explaining the Geometry, Electronic Structure, and Optical Properties of Ca ₁₀ V ₆ O ₂₅ . Inorganic Chemistry, 2018, 57, 15489-15499.	1.9	18

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19	Observation of dielectric dispersion and relaxation behavior in Ni ²⁺ -substituted cobalt ferrite nanoparticles. <i>Journal of Materials Chemistry C</i> , 2022, 10, 3418-3428.	2.7	18
20	Mechanism of photoluminescence in intrinsically disordered CaZrO ₃ crystals: First principles modeling of the excited electronic states. <i>Journal of Alloys and Compounds</i> , 2017, 722, 981-995.	2.8	16
21	Unveiling the shape-selective CoCr ₂ -yScyO ₄ nanomagnetism. <i>Applied Surface Science</i> , 2022, 574, 151555.	3.1	15
22	In Situ Growth of Bi Nanoparticles on NaBiO ₃ , $\hat{\Gamma}$, and $\hat{\Gamma}$ -Bi ₂ O ₃ Surfaces: Electron Irradiation and Theoretical Insights. <i>Journal of Physical Chemistry C</i> , 2019, 123, 5023-5030.	1.5	14
23	First principle investigation of the exposed surfaces and morphology of $\hat{\Gamma}$ -ZnMoO ₄ . <i>Journal of Applied Physics</i> , 2019, 126, 235301.	1.1	14
24	Atomistic Perspective on the Intrinsic White-Light Photoluminescence of Rare-Earth Free MgMoO ₄ Nanoparticles. <i>Crystal Growth and Design</i> , 2020, 20, 6592-6603.	1.4	13
25	Quantum mechanical modeling of Zn-based spinel oxides: Assessing the structural, vibrational, and electronic properties. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26368.	1.0	9
26	Barium strontium titanate-based perovskite materials from DFT perspective: assessing the structural, electronic, vibrational, dielectric and energetic properties. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	9
27	In situ Formation of Metal Nanoparticles through Electron Beam Irradiation: Modeling Real Materials from First-Principles Calculations. <i>Journal of Material Science & Engineering</i> , 2018, 07, .	0.2	8
28	Presence of excited electronic states on terbium incorporation in CaMoO ₄ : Insights from experimental synthesis and first-principles calculations. <i>Journal of Physics and Chemistry of Solids</i> , 2021, 149, 109790.	1.9	8
29	Magnetism and DFT calculations for understanding magnetic ground state of Fe doped Mn ₂ O ₃ . <i>Journal of Alloys and Compounds</i> , 2021, 861, 158567.	2.8	8
30	Hematite rhombuses for chemiresistive ozone sensors: Experimental and theoretical approaches. <i>Applied Surface Science</i> , 2021, 563, 150209.	3.1	8
31	Unraveling the relationship between bulk structure and exposed surfaces and its effect on the electronic structure and photoluminescent properties of Ba _{0.5} Sr _{0.5} TiO ₃ : A joint experimental and theoretical approach. <i>Materials Research Bulletin</i> , 2021, 143, 111442.	2.7	7
32	Unconventional Disorder by Femtosecond Laser Irradiation in Fe ₂ O ₃ . <i>ACS Omega</i> , 2021, 6, 28049-28062.	1.6	4
33	Light-assisted ozone gas-sensing performance of SnO ₂ nanoparticles: Experimental and theoretical insights. <i>Sensors and Actuators Reports</i> , 2022, 4, 100081.	2.3	3
34	Integration of experiment and computational modeling on the Tb doping process in CaMoO ₄ obtained by USP method: An efficient way to obtain photoluminescent materials. <i>ChemPhysChem</i> , 2020, , .	1.0	1
35	Luminescence and structural properties of Ca _{1-x} ZrO ₃ :Eux: An experimental and theoretical approach. <i>Eletica Quimica</i> , 2022, 47, 90-104.	0.2	1
36	DFT Simulations for Heterogeneous Photocatalysis from ZnO and CuO Semiconductors. <i>Engineering Materials</i> , 2021, , 185-200.	0.3	0

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37	An Ab Initio Analysis of Structural and Electronic Properties of Cubic SrSnO ₃ . <i>Orbital</i> , 2021, 13, .	0.1	0