Marisa Carvalho Oliveira

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

15 432 33 20 h-index g-index citations papers 3.89 4.1 37 599 L-index avg, IF ext. citations ext. papers

#	Paper	IF	Citations
33	Light-assisted ozone gas-sensing performance of SnO2 nanoparticles: Experimental and theoretical insights. <i>Sensors and Actuators Reports</i> , 2022 , 100081	4.7	
32	Unveiling the shape-selective CoCr2-yScyO4 nanomagnetism. <i>Applied Surface Science</i> , 2022 , 574, 15155	5 6.7	0
31	Unconventional Disorder by Femtosecond Laser Irradiation in FeO. ACS Omega, 2021, 6, 28049-28062	3.9	O
30	Magnetism and DFT calculations for understanding magnetic ground state of Fe doped Mn2O3. Journal of Alloys and Compounds, 2021, 861, 158567	5.7	1
29	Presence of excited electronic states on terbium incorporation in CaMoO4: Insights from experimental synthesis and first-principles calculations. <i>Journal of Physics and Chemistry of Solids</i> , 2021 , 149, 109790	3.9	2
28	Role of Surfaces in the Magnetic and Ozone Gas-Sensing Properties of ZnFeO Nanoparticles: Theoretical and Experimental Insights. <i>ACS Applied Materials & District Action Sensitive</i> 13, 4605-4617	9.5	16
27	DFT Simulations for Heterogeneous Photocatalysis from ZnO and CuO Semiconductors. <i>Engineering Materials</i> , 2021 , 185-200	0.4	
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	1.9	4
25	Hematite rhombuses for chemiresitive ozone sensors: Experimental and theoretical approaches. <i>Applied Surface Science</i> , 2021 , 563, 150209	6.7	2
24	Unraveling the relationship between bulk structure and exposed surfaces and its effect on the electronic structure and photoluminescent properties of Ba0.5Sr0.5TiO3: A joint experimental and theoretical approach. <i>Materials Research Bulletin</i> , 2021 , 143, 111442	5.1	2
23	Towards shape-oriented Bi-doped CoCr2O4 nanoparticles from theoretical and experimental perspectives: structural, morphological, optical, electrical and magnetic properties. <i>Journal of Materials Chemistry C</i> , 2021 , 9, 6452-6469	7.1	7
22	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	2.1	0
21	Disclosing the Structural, Electronic, Magnetic, and Morphological Properties of CuMnO2: A Unified Experimental and Theoretical Approach. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 5378-5388	3.8	16
20	Structural, electronic, vibrational and magnetic properties of Zn2+ substituted MnCr2O4 nanoparticles. <i>Journal of Magnetism and Magnetic Materials</i> , 2020 , 502, 166595	2.8	24
19	Connecting the surface structure, morphology and photocatalytic activity of Ag2O: An in depth and unified theoretical investigation. <i>Applied Surface Science</i> , 2020 , 509, 145321	6.7	29
18	Recent progress and approaches on the synthesis of Mn-doped zinc oxide nanoparticles: a theoretical and experimental investigation on the photocatalytic performance. <i>New Journal of Chemistry</i> , 2020 , 44, 8805-8812	3.6	15
17	Temperature dependence on phase evolution in the BaTiO3 polytypes studied using ab initio calculations. <i>International Journal of Quantum Chemistry</i> , 2020 , 120, e26054	2.1	7

LIST OF PUBLICATIONS

Connecting theory with experiment to understand the photocatalytic activity of CuOIInO heterostructure. <i>Ceramics International</i> , 2020 , 46, 9446-9454	5.1	24
Structural, electronic and magnetic properties of Sc3+ doped CoCr2O4 nanoparticles. <i>New Journal of Chemistry</i> , 2020 , 44, 14246-14255	3.6	16
Atomistic Perspective on the Intrinsic White-Light Photoluminescence of Rare-Earth Free MgMoO4 Nanoparticles. <i>Crystal Growth and Design</i> , 2020 , 20, 6592-6603	3.5	7
In Situ Growth of Bi Nanoparticles on NaBiO3, [] and EBi2O3 Surfaces: Electron Irradiation and Theoretical Insights. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 5023-5030	3.8	10
Geometry, electronic structure, morphology, and photoluminescence emissions of BaW1-xMoxO4 (x = 0, 0.25, 0.50, 0.75, and 1) solid solutions: Theory and experiment in concert. <i>Applied Surface Science</i> , 2019 , 463, 907-917	6.7	15
Understanding the White-Emitting CaMoO4 Co-Doped Eu3+, Tb3+, and Tm3+ Phosphor through Experiment and Computation. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 18536-18550	3.8	27
First principle investigation of the exposed surfaces and morphology of EnMoO4. <i>Journal of Applied Physics</i> , 2019 , 126, 235301	2.5	10
Structure, morphology and photoluminescence emissions of ZnMoO4: RE $3+=Tb3+-Tm3+-X$ Eu $3+(x \not\sqsubseteq 1, 1.5, 2, 2.5 \text{ and } 3 \text{ mol}\%)$ particles obtained by the sonochemical method. <i>Journal of Alloys and Compounds</i> , 2018 , 750, 55-70	5.7	26
Experimental and theoretical study of the energetic, morphological, and photoluminescence properties of CaZrO3:Eu3+. <i>CrystEngComm</i> , 2018 , 20, 5519-5530	3.3	17
Experimental and theoretical study to explain the morphology of CaMoO 4 crystals. <i>Journal of Physics and Chemistry of Solids</i> , 2018 , 114, 141-152	3.9	31
Computational Chemistry Meets Experiments for Explaining the Geometry, Electronic Structure, and Optical Properties of CaVO. <i>Inorganic Chemistry</i> , 2018 , 57, 15489-15499	5.1	15
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,	0.7	3
Mechanism of photoluminescence in intrinsically disordered CaZrO3 crystals: First principles modeling of the excited electronic states. <i>Journal of Alloys and Compounds</i> , 2017 , 722, 981-995	5.7	15
Synthesis and morphological transformation of BaWO4 crystals: Experimental and theoretical insights. <i>Ceramics International</i> , 2016 , 42, 10913-10921	5.1	40
On the morphology of BaMoO4 crystals: A theoretical and experimental approach. <i>Crystal Research and Technology</i> , 2016 , 51, 634-644	1.3	16
A theoretical investigation of the structural and electronic properties of orthorhombic CaZrO3. <i>Ceramics International</i> , 2015 , 41, 3069-3074	5.1	34
	heterostructure. <i>Ceramics International</i> , 2020 , 46, 9446-9454 Structural, electronic and magnetic properties of 5c3+ doped CoCr2O4 nanoparticles. <i>New Journal of Chemistry</i> , 2020 , 44, 14246-14255 Atomistic Perspective on the Intrinsic White-Light Photoluminescence of Rare-Earth Free MgMoO4 Nanoparticles. <i>Crystal Growth and Design</i> , 2020 , 20, 6592-6603 In Situ Growth of Bi Nanoparticles on NaBiO3, ‡ and Bi2O3 Surfaces: Electron Irradiation and Theoretical Insights. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 5023-5030 Geometry, electronic structure, morphology, and photoluminescence emissions of BaW1-xMoxO4 (x = 0, 0.25, 0.50, 0.75, and 1) solid solutions: Theory and experiment in concert. <i>Applied Surface Science</i> , 2019 , 463, 907-917 Understanding the White-Emitting CaMoO4 Co-Doped Eu3+, Tb3+, and Tm3+ Phosphor through Experiment and Computation. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 18536-18550 First principle investigation of the exposed surfaces and morphology of IZnMoO4. <i>Journal of Applied Physics</i> , 2019 , 126, 235301 Structure, morphology and photoluminescence emissions of ZnMoO4: RE 3+=Tb3+ · Tm3+ · X Eu3+ (X £ 1, 1.5, 2, 2.5 and 3 mol%) particles obtained by the sonochemical method. <i>Journal of Alloys and Compounds</i> , 2018 , 750, 55-70 Experimental and theoretical study of the energetic, morphological, and photoluminescence properties of CaZrO3:Eu3+. <i>CrystEngComm</i> , 2018 , 20, 5519-5530 Experimental and theoretical study to explain the morphology of CaMoO 4 crystals. <i>Journal of Physics and Chemistry of Solids</i> , 2018 , 114, 141-152 Computational Chemistry Meets Experiments for Explaining the Geometry, Electronic Structure, and Optical Properties of CaVO. <i>Inorganic Chemistry</i> , 2018 , 57, 15489-15499 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, Mechanism of photoluminescence in intrinsically disordered CaZrO3 crystals: F	Structural, electronic and magnetic properties of Sc3+ doped CoCr2O4 nanoparticles. New Journal of Chemistry, 2020, 44, 14246-14255 Atomistic Perspective on the Intrinsic White-Light Photoluminescence of Rare-Earth Free MgMoO4 Nanoparticles. Crystal Growth and Design, 2020, 20, 6592-6603 In Situ Growth of Bi Nanoparticles on NaBiO3, Fl and FBi2O3 Surfaces: Electron Irradiation and Theoretical Insights. Journal of Physical Chemistry, C, 2019, 123, 5023-5030 Geometry, electronic structure, morphology, and photoluminescence emissions of BaW1-xMoxO4 (x = 0, 0.25, 0.50, 0.75, and 1) solid solutions: Theory and experiment in concert. Applied Surface Science, 2019, 463, 907-917 Understanding the White-Emitting CaMoO4 Co-Doped Eu3+, Tb3+, and Tm3+ Phosphor through Experiment and Computation. Journal of Physical Chemistry C, 2019, 123, 18536-18550 3.8 First principle investigation of the exposed surfaces and morphology of EZnMoO4. Journal of Applied Physics, 2019, 126, 235301 5.7 Structure, morphology and photoluminescence emissions of ZnMoO4: RE 3+=Tb3+-Tm3+-X Eu3+ (xi=1,1.5, 2, 2.5 and 3 mol%) particles obtained by the sonochemical method. Journal of Alloys and Compounds, 2018, 750, 55-70 Experimental and theoretical study of the energetic, morphological, and photoluminescence properties of CaZrO3:Eu3+. CrystEngComm, 2018, 20, 5519-5530 Experimental and theoretical study to explain the morphology of CaMoO 4 crystals. Journal of Physics and Chemistry of Solids. 2018, 114, 141-152 Computational Chemistry Meets Experiments for Explaining the Geometry, Electronic Structure, and Optical Properties of CaVO. Inorganic Chemistry, 2018, 57, 15489-15499 In situ Formation of Metal Nanoparticles through Electron Beam Irradiation: Modeling Real Materials from First-Principles Calculations. Journal of Material Science & Engineering, 2018, 07, 97 Mechanism of photoluminescence in intrinsically disordered CaZrO3 crystals: First principles modeling of the excited electronic states. Journal of Alloys and Compounds, 2017, 7