

# Lourdes Gracia

## List of Publications by Citations

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104  
papers

3,143  
citations

35  
h-index

49  
g-index

106  
ext. papers

3,498  
ext. citations

3.7  
avg, IF

5.21  
L-index

#	Paper	IF	Citations
104	Toward an Understanding of the Growth of Ag Filaments on $\beta$ -Ag <sub>2</sub> WO <sub>4</sub> and Their Photoluminescent Properties: A Combined Experimental and Theoretical Study. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 1229-1239	3.8	111
103	Facet-dependent photocatalytic and antibacterial properties of $\beta$ -Ag <sub>2</sub> WO <sub>4</sub> crystals: combining experimental data and theoretical insights. <i>Catalysis Science and Technology</i> , <b>2015</b> , 5, 4091-4107	5.5	110
102	Density functional theory study of the brookite surfaces and phase transitions between natural titania polymorphs. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 23417-23	3.4	103
101	Experimental and Theoretical Study on the Structure, Optical Properties, and Growth of Metallic Silver Nanostructures in Ag <sub>3</sub> PO <sub>4</sub> . <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 6293-6306	3.8	92
100	ZnWO nanocrystals: synthesis, morphology, photoluminescence and photocatalytic properties. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 1923-1937	3.6	77
99	Structural and electronic analysis of the atomic scale nucleation of Ag on $\beta$ -Ag <sub>2</sub> WO <sub>4</sub> induced by electron irradiation. <i>Scientific Reports</i> , <b>2014</b> , 4, 5391	4.9	76
98	Presence of excited electronic state in CaWO <sub>4</sub> crystals provoked by a tetrahedral distortion: An experimental and theoretical investigation. <i>Journal of Applied Physics</i> , <b>2011</b> , 110, 043501	2.5	74
97	Effects of surface stability on the morphological transformation of metals and metal oxides as investigated by first-principles calculations. <i>Nanotechnology</i> , <b>2015</b> , 26, 405703	3.4	70
96	Toward Understanding the Photocatalytic Activity of PbMoO <sub>4</sub> Powders with Predominant (111), (100), (011), and (110) Facets. A Combined Experimental and Theoretical Study. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 21382-21395	3.8	69
95	Theoretical Study on the Molecular Mechanism for the Reaction of VO <sub>2</sub> <sup>+</sup> with C <sub>2</sub> H <sub>4</sub> . <i>Journal of Physical Chemistry A</i> , <b>2003</b> , 107, 3107-3120	2.8	68
94	A Joint Experimental and Theoretical Study on the Nanomorphology of CaWO <sub>4</sub> Crystals. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 20113-20119	3.8	66
93	Characterization of the high-pressure structures and phase transformations in SnO <sub>2</sub> . A density functional theory study. <i>Journal of Physical Chemistry B</i> , <b>2007</b> , 111, 6479-85	3.4	65
92	DFT Study of the Reaction between VO <sub>2</sub> <sup>+</sup> and C <sub>2</sub> H <sub>6</sub> . <i>Organometallics</i> , <b>2004</b> , 23, 730-739	3.8	61
91	High-pressure study of the behavior of mineral barite by x-ray diffraction. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	59
90	Structural and vibrational study of cubic Sb <sub>2</sub> O <sub>3</sub> under high pressure. <i>Physical Review B</i> , <b>2012</b> , 85,	3.3	57
89	Chemical structure and reactivity by means of quantum chemical topology analysis. <i>Computational and Theoretical Chemistry</i> , <b>2015</b> , 1053, 17-30	2	53
88	Photoluminescence and Photocatalytic Properties of Ag PO Microcrystals: An Experimental and Theoretical Investigation. <i>ChemPlusChem</i> , <b>2016</b> , 81, 202-212	2.8	52

87	Elucidating the real-time Ag nanoparticle growth on $\text{Ag}_2\text{WO}_4$ during electron beam irradiation: experimental evidence and theoretical insights. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 5352-9	3.6	52
86	Identifying and rationalizing the morphological, structural, and optical properties of [Formula: see text]-AgMoO microcrystals, and the formation process of Ag nanoparticles on their surfaces: combining experimental data and first-principles calculations. <i>Science and Technology of Advanced Materials</i> , <b>2015</b> , 16, 065002	7.1	52
85	Compression of scheelite-type $\text{SrMoO}_4$ under quasi-hydrostatic conditions: Redefining the high-pressure structural sequence. <i>Journal of Applied Physics</i> , <b>2013</b> , 113, 123510	2.5	52
84	Mechanism of Antibacterial Activity via Morphology Change of $\text{AgVO}$ : Theoretical and Experimental Insights. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2017</b> , 9, 11472-11481	9.5	46
83	A 3D platform for the morphology modulation of materials: first principles calculations on the thermodynamic stability and surface structure of metal oxides: $\text{Co}_3\text{O}_4$ , $\text{Fe}_2\text{O}_3$ , and $\text{In}_2\text{O}_3$ . <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2016</b> , 24, 025007	2	46
82	Surfactant-Mediated Morphology and Photocatalytic Activity of $\text{Ag}_2\text{WO}_4$ Material. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 8667-8679	3.8	45
81	First-Principles Study of Pressure-Induced Phase Transitions and Electronic Properties of $\text{Ag}_2\text{MoO}_4$ . <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 3724-3732	3.8	42
80	A Combined Experimental and Theoretical Study on the Formation of Ag Filaments on $\text{Ag}_2\text{MoO}_4$ Induced by Electron Irradiation. <i>Particle and Particle Systems Characterization</i> , <b>2015</b> , 32, 646-651	3.1	41
79	A theoretical study on the photoluminescence of $\text{SrTiO}_3$ . <i>Chemical Physics Letters</i> , <b>2010</b> , 493, 141-146	2.5	41
78	Insight into the Effects of Fe Addition on the Local Structure and Electronic Properties of $\text{SrTiO}_3$ . <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 4930-4940	3.8	40
77	Characterization of the $\text{TiSiO}_4$ structure and its pressure-induced phase transformations: Density functional theory study. <i>Physical Review B</i> , <b>2009</b> , 80,	3.3	40
76	Synthesis and morphological transformation of $\text{BaWO}_4$ crystals: Experimental and theoretical insights. <i>Ceramics International</i> , <b>2016</b> , 42, 10913-10921	5.1	40
75	Synthesis, antifungal evaluation and optical properties of silver molybdate microcrystals in different solvents: a combined experimental and theoretical study. <i>Dalton Transactions</i> , <b>2016</b> , 45, 10736-43	4.3	38
74	Migration of the subsurface C impurity in $\text{Pd}(111)$ . <i>Physical Review B</i> , <b>2005</b> , 71,	3.3	38
73	Quantum-mechanical simulation of $\text{MgAl}_2\text{O}_4$ under high pressure. <i>Physical Review B</i> , <b>2002</b> , 66,	3.3	37
72	An Experimental and Computational Study of $\text{AgVO}_3$ : Optical Properties and Formation of Ag Nanoparticles. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 12254-12264	3.8	37
71	Photoluminescent properties of $\text{ZrO}_2$ : $\text{Tm}^{3+}$ , $\text{Tb}^{3+}$ , $\text{Eu}^{3+}$ powders: A combined experimental and theoretical study. <i>Journal of Alloys and Compounds</i> , <b>2017</b> , 695, 3094-3103	5.7	36
70	$\text{CaSO}_4$ and its pressure-induced phase transitions. A density functional theory study. <i>Inorganic Chemistry</i> , <b>2012</b> , 51, 1751-9	5.1	36

69	Experimental and theoretical investigation of ThGeO <sub>4</sub> at high pressure. <i>Physical Review B</i> , <b>2009</b> , 80,	3.3	35
68	An experimental and theoretical investigation on the optical and photocatalytic properties of ZnS nanoparticles. <i>Journal of Physics and Chemistry of Solids</i> , <b>2017</b> , 103, 179-189	3.9	33
67	Formation of Ag Nanoparticles on $\beta$ -Ag <sub>2</sub> WO <sub>4</sub> through Electron Beam Irradiation: A Synergetic Computational and Experimental Study. <i>Inorganic Chemistry</i> , <b>2016</b> , 55, 8661-71	5.1	33
66	Experimental and Theoretical Study of Bi <sub>2</sub> O <sub>2</sub> Se Under Compression. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 8853-8867	3.8	32
65	In situ Transmission Electron Microscopy observation of Ag nanocrystal evolution by surfactant free electron-driven synthesis. <i>Scientific Reports</i> , <b>2016</b> , 6, 21498	4.9	32
64	A DFT Study of Structural and Electronic Properties of ZnS Polymorphs and its Pressure-Induced Phase Transitions. <i>Journal of the American Ceramic Society</i> , <b>2014</b> , 97, 4011-4018	3.8	31
63	Experimental and theoretical study to explain the morphology of CaMoO <sub>4</sub> crystals. <i>Journal of Physics and Chemistry of Solids</i> , <b>2018</b> , 114, 141-152	3.9	31
62	Theoretical approach for determining the relation between the morphology and surface magnetism of Co <sub>3</sub> O <sub>4</sub> . <i>Journal of Magnetism and Magnetic Materials</i> , <b>2018</b> , 453, 262-267	2.8	30
61	A Theoretical Study on the Pressure-Induced Phase Transitions in the Inverse Spinel Structure Zn <sub>2</sub> SnO <sub>4</sub> . <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 7740-7746	3.8	28
60	Mechanistic Insights into the Reaction between VO <sub>2</sub> <sup>+</sup> and Propene Based on a DFT Study. <i>Organometallics</i> , <b>2006</b> , 25, 1643-1653	3.8	28
59	In situ growth of Ag nanoparticles on $\beta$ -Ag <sub>2</sub> WO <sub>4</sub> under electron irradiation: probing the physical principles. <i>Nanotechnology</i> , <b>2016</b> , 27, 225703	3.4	28
58	Understanding the White-Emitting CaMoO <sub>4</sub> Co-Doped Eu <sup>3+</sup> , Tb <sup>3+</sup> , and Tm <sup>3+</sup> Phosphor through Experiment and Computation. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 18536-18550	3.8	27
57	Structural study of $\beta$ -Bi <sub>2</sub> O <sub>3</sub> under pressure. <i>Journal of Physics Condensed Matter</i> , <b>2013</b> , 25, 475402	1.8	27
56	Structural and Electronic Effects of Incorporating Mn in TiO <sub>2</sub> Films Grown by Sputtering: Anatase versus Rutile. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 8753-8762	3.8	27
55	Theoretical and Experimental Insight on Ag <sub>2</sub> CrO <sub>4</sub> Microcrystals: Synthesis, Characterization, and Photoluminescence Properties. <i>Inorganic Chemistry</i> , <b>2016</b> , 55, 8961-70	5.1	27
54	Structure, morphology and photoluminescence emissions of ZnMoO <sub>4</sub> : RE <sup>3+</sup> =Tb <sup>3+</sup> - Tm <sup>3+</sup> - X Eu <sup>3+</sup> (x= 1, 1.5, 2, 2.5 and 3 mol%) particles obtained by the sonochemical method. <i>Journal of Alloys and Compounds</i> , <b>2018</b> , 750, 55-70	5.7	26
53	A theoretical study on the electronic structure of Au-XO(0,-1,+1) (X=C, N, and O) complexes: effect of an external electric field. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 13255-63	2.8	25
52	DFT study of the water-assisted tautomerization process between hydrated oxide, MO(H <sub>2</sub> O) <sup>+</sup> , and dihydroxide, M(OH) <sub>2</sub> <sup>+</sup> , cations (M=V, Nb and Ta). <i>Chemical Physics Letters</i> , <b>2004</b> , 384, 56-62	2.5	24

51	A Theoretical Study on the Gas Phase Reactions of the Anions NbO <sub>3</sub> <sup>-</sup> , NbO <sub>5</sub> <sup>-</sup> , and NbO <sub>2</sub> (OH) <sub>2</sub> <sup>-</sup> with H <sub>2</sub> O and O <sub>2</sub> . <i>Journal of Physical Chemistry A</i> , <b>2004</b> , 108, 10850-10860	2.8	24
50	Unveiling the role of $\delta$ -Ag <sub>2</sub> MoO <sub>4</sub> microcrystals to the improvement of antibacterial activity. <i>Materials Science and Engineering C</i> , <b>2020</b> , 111, 110765	8.3	23
49	Intercalation processes and diffusion paths of lithium ions in spinel-type structured Li <sub>1+x</sub> Ti <sub>2</sub> O <sub>4</sub> : Density functional theory study. <i>Physical Review B</i> , <b>2008</b> , 77,	3.3	22
48	Understanding the formation and growth of Ag nanoparticles on silver chromate induced by electron irradiation in electron microscope: A combined experimental and theoretical study. <i>Journal of Solid State Chemistry</i> , <b>2016</b> , 239, 220-227	3.3	21
47	Pressure-induced phase transitions in AgClO <sub>4</sub> . <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	20
46	First-Principles Study on Polymorphs of AgVO <sub>3</sub> : Assessing to Structural Stabilities and Pressure-Induced Transitions. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 27624-27642	3.8	19
45	Electronic structure and magnetic properties of FeWO <sub>4</sub> nanocrystals synthesized by the microwave-hydrothermal method. <i>Materials Characterization</i> , <b>2012</b> , 73, 124-129	3.9	19
44	Unraveling the Mechanisms of the Selective Oxidation of Methanol to Formaldehyde in Vanadia Supported on Titania Catalyst. <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 6039-6046	3.8	19
43	A joint experimental and theoretical study on the electronic structure and photoluminescence properties of Al <sub>2</sub> (WO <sub>4</sub> ) <sub>3</sub> powders. <i>Journal of Molecular Structure</i> , <b>2015</b> , 1081, 381-388	3.4	18
42	Synthesis and characterization of metastable $\delta$ -Ag <sub>2</sub> WO <sub>4</sub> : an experimental and theoretical approach. <i>Dalton Transactions</i> , <b>2016</b> , 45, 1185-91	4.3	18
41	Uncovering the metastable $\delta$ -Ag <sub>2</sub> WO <sub>4</sub> phase: a joint experimental and theoretical study. <i>RSC Advances</i> , <b>2017</b> , 7, 5610-5620	3.7	18
40	Synthesis, optical and ferroelectric properties of PZT thin films: experimental and theoretical investigation. <i>Journal of Materials Chemistry</i> , <b>2012</b> , 22, 6587		18
39	Formation of Ag nanoparticles under electron beam irradiation: Atomistic origins from first-principles calculations. <i>International Journal of Quantum Chemistry</i> , <b>2018</b> , 118, e25551	2.1	18
38	Experimental and theoretical study of the energetic, morphological, and photoluminescence properties of CaZrO <sub>3</sub> :Eu <sup>3+</sup> . <i>CrystEngComm</i> , <b>2018</b> , 20, 5519-5530	3.3	17
37	A DFT study of methanol dissociation on isolated vanadate groups. <i>Catalysis Today</i> , <b>2008</b> , 139, 214-220	5.3	16
36	High-pressure behaviour of selenium-based spinels and related structures—experimental and theoretical study. <i>Journal of Physics Condensed Matter</i> , <b>2004</b> , 16, 53-63	1.8	16
35	Effects of chemical substitution on the structural and optical properties of $\delta$ -Ag <sub>2-2x</sub> Ni <sub>x</sub> WO <sub>4</sub> (0 ≤ x ≤ 0.08) solid solutions. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 21966-75	3.6	16
34	On the morphology of BaMoO <sub>4</sub> crystals: A theoretical and experimental approach. <i>Crystal Research and Technology</i> , <b>2016</b> , 51, 634-644	1.3	16

33	Geometry, electronic structure, morphology, and photoluminescence emissions of BaW <sub>1-x</sub> MoxO <sub>4</sub> (x = 0, 0.25, 0.50, 0.75, and 1) solid solutions: Theory and experiment in concert. <i>Applied Surface Science</i> , <b>2019</b> , 463, 907-917	6.7	15
32	Joint Theoretical and Experimental Study on the La Doping Process in InO: Phase Transition and Electrocatalytic Activity. <i>Inorganic Chemistry</i> , <b>2019</b> , 58, 11738-11750	5.1	15
31	Quantum mechanical modeling of excited electronic states and their relationship to cathodoluminescence of BaZrO <sub>3</sub> . <i>Journal of Applied Physics</i> , <b>2013</b> , 114, 043714	2.5	15
30	Mechanism of photoluminescence in intrinsically disordered CaZrO <sub>3</sub> crystals: First principles modeling of the excited electronic states. <i>Journal of Alloys and Compounds</i> , <b>2017</b> , 722, 981-995	5.7	15
29	Theoretical study on the reaction mechanism of VO <sub>2</sub> <sup>+</sup> with propyne in gas phase. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 1808-16	2.8	15
28	Computational Chemistry Meets Experiments for Explaining the Geometry, Electronic Structure, and Optical Properties of CaVO. <i>Inorganic Chemistry</i> , <b>2018</b> , 57, 15489-15499	5.1	15
27	Structural and Electronic Properties of Lithiated SnO <sub>2</sub> . A Periodic DFT Study. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 16127-16137	3.8	14
26	∅ and ∅AgVO <sub>3</sub> polymorphs as photoluminescent materials: An example of temperature-driven synthesis. <i>Ceramics International</i> , <b>2018</b> , 44, 5939-5944	5.1	13
25	Disclosing the electronic structure and optical properties of Ag <sub>4</sub> V <sub>2</sub> O <sub>7</sub> crystals: experimental and theoretical insights. <i>CrystEngComm</i> , <b>2016</b> , 18, 6483-6491	3.3	13
24	Density functional theory study of the oxidation of methanol to formaldehyde on a hydrated vanadia cluster. <i>Journal of Computational Chemistry</i> , <b>2010</b> , 31, 2493-501	3.5	11
23	Polymorphs of ZnV <sub>2</sub> O <sub>6</sub> under Pressure: A First-Principle Investigation. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 3239-3253	3.8	11
22	In Situ Growth of Bi Nanoparticles on NaBiO <sub>3</sub> , ∅ and ∅Bi <sub>2</sub> O <sub>3</sub> Surfaces: Electron Irradiation and Theoretical Insights. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 5023-5030	3.8	10
21	First principle investigation of the exposed surfaces and morphology of ∅ZnMoO <sub>4</sub> . <i>Journal of Applied Physics</i> , <b>2019</b> , 126, 235301	2.5	10
20	Composition Dependence of the Energy Barrier for Lithium Diffusion in Amorphous WO <sub>3</sub> . <i>Electrochemical and Solid-State Letters</i> , <b>2005</b> , 8, J21		9
19	Prediction of dopant atom distribution on nanocrystals using thermodynamic arguments. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 1089-94	3.6	8
18	Selective Synthesis of ∅ ∅ and ∅AgWO Polymorphs: Promising Platforms for Photocatalytic and Antibacterial Materials. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 1062-1079	5.1	8
17	Structure, electronic properties, morphology evolution, and photocatalytic activity in PbMoO and PbCaSrMoO (= 0.1, 0.2, 0.3, 0.4 and 0.5) solid solutions. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 25876-25891	3.6	8
16	Modulating the properties of multifunctional semiconductors by means of morphology: Theory meets experiments. <i>Computational Materials Science</i> , <b>2021</b> , 188, 110217	3.2	8

15	Bonding and compressibility in molecular and polymeric phases of solid CO <sub>2</sub> . <i>Journal of Physics Condensed Matter</i> , <b>2004</b> , 16, S1263-S1270	1.8	7
14	Efficient Ni and Fe doping process in ZnO with enhanced photocatalytic activity: A theoretical and experimental investigation. <i>Materials Research Bulletin</i> , <b>2022</b> , 111849	5.1	6
13	Bonding changes across the Cristobalite-stishovite transition path in silica. <i>High Pressure Research</i> , <b>2009</b> , 29, 93-96	1.6	5
12	DFT study on the water-assisted mechanism for the reaction between VO <sup>+</sup> and NH <sub>3</sub> to yield VNH <sup>+</sup> and H <sub>2</sub> O. <i>Chemical Physics Letters</i> , <b>2006</b> , 427, 265-270	2.5	5
11	Synthesis of Cuboctahedral CeO <sub>2</sub> Nanoclusters and Their Assembly into Cuboid Nanoparticles by Oriented Attachment. <i>ChemNanoMat</i> , <b>2017</b> , 3, 228-232	3.5	4
10	Identifying and explaining vibrational modes of sanbornite (low-BaSiO) and BaSiO: A joint experimental and theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , <b>2021</b> , 248, 119130	4.4	3
9	Density-functional study of pressure-induced phase transitions and electronic properties of ZnVO <sub>2</sub> . <i>RSC Advances</i> , <b>2021</b> , 11, 10401-10415	3.7	3
8	In situ Formation of Metal Nanoparticles through Electron Beam Irradiation: Modeling Real Materials from First-Principles Calculations. <i>Journal of Material Science &amp; Engineering</i> , <b>2018</b> , 07,	0.7	3
7	Bridging Structure and Real-Space Topology: Understanding Complex Molecules and Solid-State Materials <b>2017</b> , 427-454		2
6	Stability of MgAl <sub>2</sub> O <sub>4</sub> Under High-Pressure Conditions. <i>High Pressure Research</i> , <b>2002</b> , 22, 447-450	1.6	2
5	Quantum Chemical Topology Approach for Dissecting Chemical Structure and Reactivity. <i>Challenges and Advances in Computational Chemistry and Physics</i> , <b>2016</b> , 257-294	0.7	2
4	Towards a white-emitting phosphor Ca <sub>10</sub> V <sub>6</sub> O <sub>25</sub> based material. <i>Journal of Luminescence</i> , <b>2020</b> , 220, 116990	3.8	2
3	Ag <sub>2</sub> WO <sub>4</sub> under microwave, electron beam and femtosecond laser irradiations: Unveiling the relationship between morphology and photoluminescence emissions. <i>Journal of Alloys and Compounds</i> , <b>2022</b> , 903, 163840	5.7	1
2	Integrated experimental and theoretical study on the phase transition and photoluminescent properties of ZrO <sub>2</sub> :xTb <sup>3+</sup> (x=1, 2, 4 and 8 mol %). <i>Materials Research Bulletin</i> , <b>2022</b> , 145, 111532	5.1	0
1	Chemical Bonding under Pressure <b>2015</b> , 131-157		