Lourdes Gracia

List of Publications by Year in Descending Order

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	Ag2WO4 under microwave, electron beam and femtosecond laser irradiations: Unveiling the relationship between morphology and photoluminescence emissions. *Journal of Alloys and Compounds*, **2022**, 903, 163840	5.7	1
103	Integrated experimental and theoretical study on the phase transition and photoluminescent properties of ZrO2:xTb3+ (x=1, 2, 4 and 8 mol %). *Materials Research Bulletin*, **2022**, 145, 111532	5.1	0
102	Efficient Ni and Fe doping process in ZnO with enhanced photocatalytic activity: A theoretical and experimental investigation. *Materials Research Bulletin*, **2022**, 111849	5.1	6
101	Selective Synthesis of and AgWO Polymorphs: Promising Platforms for Photocatalytic and Antibacterial Materials. *Inorganic Chemistry*, **2021**, 60, 1062-1079	5.1	8
100	Identifying and explaining vibrational modes of sanbornite (low-BaSiO) and BaSiO: A joint experimental and theoretical study. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 248, 119130	4.4	3
99	Modulating the properties of multifunctional semiconductors by means of morphology: Theory meets experiments. *Computational Materials Science*, **2021**, 188, 110217	3.2	8
98	Density-functional study of pressure-induced phase transitions and electronic properties of ZnVO.. *RSC Advances*, **2021**, 11, 10401-10415	3.7	3
97	Unvealing the role of AgMoO microcrystals to the improvement of antibacterial activity. *Materials Science and Engineering C*, **2020**, 111, 110765	8.3	23
96	Towards a white-emitting phosphor Ca10V6O25 based material. *Journal of Luminescence*, **2020**, 220, 116990	3.8	2
95	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. *Physical Chemistry Chemical Physics*, **2020**, 22, 25876-25891	3.6	8
94	In Situ Growth of Bi Nanoparticles on NaBiO3, and Bi2O3 Surfaces: Electron Irradiation and Theoretical Insights. *Journal of Physical Chemistry C*, **2019**, 123, 5023-5030	3.8	10
93	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	6.7	15
92	Joint Theoretical and Experimental Study on the La Doping Process in InO: Phase Transition and Electrocatalytic Activity. *Inorganic Chemistry*, **2019**, 58, 11738-11750	5.1	15
91	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	27
90	First principle investigation of the exposed surfaces and morphology of ZnMoO4. *Journal of Applied Physics*, **2019**, 126, 235301	2.5	10
89	Polymorphs of ZnV2O6 under Pressure: A First-Principle Investigation. *Journal of Physical Chemistry C*, **2019**, 123, 3239-3253	3.8	11
88	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. *Journal of Alloys and Compounds*, **2018**, 750, 55-70	5.7	26

87	Experimental and Theoretical Study of Bi2O2Se Under Compression. *Journal of Physical Chemistry C* , **2018**, 122, 8853-8867	3.8	32
86	ZnWO nanocrystals: synthesis, morphology, photoluminescence and photocatalytic properties. *Physical Chemistry Chemical Physics*, **2018**, 20, 1923-1937	3.6	77
85	and AgVO3 polymorphs as photoluminescent materials: An example of temperature-driven synthesis. *Ceramics International*, **2018**, 44, 5939-5944	5.1	13
84	Surfactant-Mediated Morphology and Photocatalytic Activity of Ag2WO4 Material. *Journal of Physical Chemistry C*, **2018**, 122, 8667-8679	3.8	45
83	Experimental and theoretical study of the energetic, morphological, and photoluminescence properties of CaZrO3:Eu3+. *CrystEngComm*, **2018**, 20, 5519-5530	3.3	17
82	Experimental and theoretical study to explain the morphology of CaMoO 4 crystals. *Journal of Physics and Chemistry of Solids*, **2018**, 114, 141-152	3.9	31
81	Formation of Ag nanoparticles under electron beam irradiation: Atomistic origins from first-principles calculations. *International Journal of Quantum Chemistry*, **2018**, 118, e25551	2.1	18
80	Theoretical approach for determining the relation between the morphology and surface magnetism of Co3O4. *Journal of Magnetism and Magnetic Materials*, **2018**, 453, 262-267	2.8	30
79	Computational Chemistry Meets Experiments for Explaining the Geometry, Electronic Structure, and Optical Properties of CaVO. *Inorganic Chemistry*, **2018**, 57, 15489-15499	5.1	15
78	In situ Formation of Metal Nanoparticles through Electron Beam Irradiation: Modeling Real Materials from First-Principles Calculations. *Journal of Material Science & Engineering*, **2018**, 07,	0.7	3
77	Synthesis of Cuboctahedral CeO2 Nanoclusters and Their Assembly into Cuboid Nanoparticles by Oriented Attachment. *ChemNanoMat*, **2017**, 3, 228-232	3.5	4
76	Mechanism of Antibacterial Activity via Morphology Change of AgVO: Theoretical and Experimental Insights. *ACS Applied Materials & Interfaces*, **2017**, 9, 11472-11481	9.5	46
75	An experimental and theoretical investigation on the optical and photocatalytic properties of ZnS nanoparticles. *Journal of Physics and Chemistry of Solids*, **2017**, 103, 179-189	3.9	33
74	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
73	Bridging Structure and Real-Space Topology: Understanding Complex Molecules and Solid-State Materials **2017**, 427-454		2
72	Mechanism of photoluminescence in intrinsically disordered CaZrO3 crystals: First principles modeling of the excited electronic states. *Journal of Alloys and Compounds*, **2017**, 722, 981-995	5.7	15
71	Uncovering the metastable Ag2WO4 phase: a joint experimental and theoretical study. *RSC Advances*, **2017**, 7, 5610-5620	3.7	18
70	Photoluminescent properties of ZrO2: Tm3+, Tb3+, Eu3+ powders: A combined experimental and theoretical study. *Journal of Alloys and Compounds*, **2017**, 695, 3094-3103	5.7	36

69	Formation of Ag Nanoparticles on Ag2WO4 through Electron Beam Irradiation: A Synergetic Computational and Experimental Study. *Inorganic Chemistry*, **2016**, 55, 8661-71	5.1	33
68	In situ Transmission Electron Microscopy observation of Ag nanocrystal evolution by surfactant free electron-driven synthesis. *Scientific Reports*, **2016**, 6, 21498	4.9	32
67	Photoluminescence and Photocatalytic Properties of Ag PO Microcrystals: An Experimental and Theoretical Investigation. *ChemPlusChem*, **2016**, 81, 202-212	2.8	52
66	Synthesis, antifungal evaluation and optical properties of silver molybdate microcrystals in different solvents: a combined experimental and theoretical study. *Dalton Transactions*, **2016**, 45, 10736-43	4.3	38
65	A 3D platform for the morphology modulation of materials: first principles calculations on the thermodynamic stability and surface structure of metal oxides: Co3O4,Fe2O3, and In2O3. *Modelling and Simulation in Materials Science and Engineering*, **2016**, 24, 025007	2	46
64	Synthesis and characterization of metastable Ag2WO4: an experimental and theoretical approach. *Dalton Transactions*, **2016**, 45, 1185-91	4.3	18
63	Quantum Chemical Topology Approach for Dissecting Chemical Structure and Reactivity. *Challenges and Advances in Computational Chemistry and Physics*, **2016**, 257-294	0.7	2
62	Disclosing the electronic structure and optical properties of Ag4V2O7 crystals: experimental and theoretical insights. *CrystEngComm*, **2016**, 18, 6483-6491	3.3	13
61	Effects of chemical substitution on the structural and optical properties of Ag2-2xNixWO4 (0 x 0.08) solid solutions. *Physical Chemistry Chemical Physics*, **2016**, 18, 21966-75	3.6	16
60	An Experimental and Computational Study of AgVO3: Optical Properties and Formation of Ag Nanoparticles. *Journal of Physical Chemistry C*, **2016**, 120, 12254-12264	3.8	37
59	In situ growth of Ag nanoparticles on Ag2WO4 under electron irradiation: probing the physical principles. *Nanotechnology*, **2016**, 27, 225703	3.4	28
58	Understanding the formation and growth of Ag nanoparticles on silver chromate induced by electron irradiation in electron microscope: A combined experimental and theoretical study. *Journal of Solid State Chemistry*, **2016**, 239, 220-227	3.3	21
57	Synthesis and morphological transformation of BaWO4 crystals: Experimental and theoretical insights. *Ceramics International*, **2016**, 42, 10913-10921	5.1	40
56	On the morphology of BaMoO4 crystals: A theoretical and experimental approach. *Crystal Research and Technology*, **2016**, 51, 634-644	1.3	16
55	Theoretical and Experimental Insight on Ag2CrO4 Microcrystals: Synthesis, Characterization, and Photoluminescence Properties. *Inorganic Chemistry*, **2016**, 55, 8961-70	5.1	27
54	A joint experimental and theoretical study on the electronic structure and photoluminescence properties of Al2(WO4)3 powders. *Journal of Molecular Structure*, **2015**, 1081, 381-388	3.4	18
53	Experimental and Theoretical Study on the Structure, Optical Properties, and Growth of Metallic Silver Nanostructures in Ag3PO4. *Journal of Physical Chemistry C*, **2015**, 119, 6293-6306	3.8	92
52	Chemical structure and reactivity by means of quantum chemical topology analysis. *Computational and Theoretical Chemistry*, **2015**, 1053, 17-30	2	53

51	Chemical Bonding under Pressure **2015**, 131-157		
50	A Combined Experimental and Theoretical Study on the Formation of Ag Filaments on Ag2MoO4 Induced by Electron Irradiation. *Particle and Particle Systems Characterization*, **2015**, 32, 646-651	3.1	41
49	Effects of surface stability on the morphological transformation of metals and metal oxides as investigated by first-principles calculations. *Nanotechnology*, **2015**, 26, 405703	3.4	70
48	Facet-dependent photocatalytic and antibacterial properties of Ag2WO4 crystals: combining experimental data and theoretical insights. *Catalysis Science and Technology*, **2015**, 5, 4091-4107	5.5	110
47	Elucidating the real-time Ag nanoparticle growth on Ag2WO4 during electron beam irradiation: experimental evidence and theoretical insights. *Physical Chemistry Chemical Physics*, **2015**, 17, 5352-9	3.6	52
46	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. *Science and Technology of Advanced Materials*, **2015**, 16, 065002	7.1	52
45	Structural and electronic analysis of the atomic scale nucleation of Ag on Ag2WO4 induced by electron irradiation. *Scientific Reports*, **2014**, 4, 5391	4.9	76
44	Prediction of dopant atom distribution on nanocrystals using thermodynamic arguments. *Physical Chemistry Chemical Physics*, **2014**, 16, 1089-94	3.6	8
43	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
42	A DFT Study of Structural and Electronic Properties of ZnS Polymorphs and its Pressure-Induced Phase Transitions. *Journal of the American Ceramic Society*, **2014**, 97, 4011-4018	3.8	31
41	Toward an Understanding of the Growth of Ag Filaments on Ag2WO4 and Their Photoluminescent Properties: A Combined Experimental and Theoretical Study. *Journal of Physical Chemistry C*, **2014**, 118, 1229-1239	3.8	111
40	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
39	Quantum mechanical modeling of excited electronic states and their relationship to cathodoluminescence of BaZrO3. *Journal of Applied Physics*, **2013**, 114, 043714	2.5	15
38	Structural study of Bi2O3 under pressure. *Journal of Physics Condensed Matter*, **2013**, 25, 475402	1.8	27
37	Toward Understanding the Photocatalytic Activity of PbMoO4 Powders with Predominant (111), (100), (011), and (110) Facets. A Combined Experimental and Theoretical Study. *Journal of Physical Chemistry C*, **2013**, 117, 21382-21395	3.8	69
36	Compression of scheelite-type SrMoO4 under quasi-hydrostatic conditions: Redefining the high-pressure structural sequence. *Journal of Applied Physics*, **2013**, 113, 123510	2.5	52
35	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
34	Structural and Electronic Properties of Lithiated SnO2. A Periodic DFT Study. *Journal of Physical Chemistry C*, **2012**, 116, 16127-16137	3.8	14

33	CaSO4 and its pressure-induced phase transitions. A density functional theory study. *Inorganic Chemistry*, **2012**, 51, 1751-9	5.1	36
32	Electronic structure and magnetic properties of FeWO4 nanocrystals synthesized by the microwave-hydrothermal method. *Materials Characterization*, **2012**, 73, 124-129	3.9	19
31	Synthesis, optical and ferroelectric properties of PZT thin films: experimental and theoretical investigation. *Journal of Materials Chemistry*, **2012**, 22, 6587		18
30	Structural and vibrational study of cubic Sb2O3 under high pressure. *Physical Review B*, **2012**, 85,	3.3	57
29	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
28	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
27	A Joint Experimental and Theoretical Study on the Nanomorphology of CaWO4 Crystals. *Journal of Physical Chemistry C*, **2011**, 115, 20113-20119	3.8	66
26	Pressure-induced phase transitions in AgClO4. *Physical Review B*, **2011**, 84,	3.3	20
25	High-pressure study of the behavior of mineral barite by x-ray diffraction. *Physical Review B*, **2011**, 84,	3.3	59
24	Unraveling the Mechanisms of the Selective Oxidation of Methanol to Formaldehyde in Vanadia Supported on Titania Catalyst. *Journal of Physical Chemistry C*, **2010**, 114, 6039-6046	3.8	19
23	A theoretical study on the photoluminescence of SrTiO3. *Chemical Physics Letters*, **2010**, 493, 141-146	2.5	41
22	Density functional theory study of the oxidation of methanol to formaldehyde on a hydrated vanadia cluster. *Journal of Computational Chemistry*, **2010**, 31, 2493-501	3.5	11
21	Experimental and theoretical investigation of ThGeO4 at high pressure. *Physical Review B*, **2009**, 80,	3.3	35
20	Characterization of the TiSiO4 structure and its pressure-induced phase transformations: Density functional theory study. *Physical Review B*, **2009**, 80,	3.3	40
19	Bonding changes across the □ristobalite-s□tishovite transition path in silica. *High Pressure Research*, **2009**, 29, 93-96	1.6	5
18	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
17	Theoretical study on the reaction mechanism of VO2+ with propyne in gas phase. *Journal of Physical Chemistry A*, **2008**, 112, 1808-16	2.8	15
16	A DFT study of methanol dissociation on isolated vanadate groups. *Catalysis Today*, **2008**, 139, 214-220	5.3	16

15	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. *Journal of Physical Chemistry A*, **2007**, 111, 13255-63	2.8	25
14	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
13	Mechanistic Insights into the Reaction between VO2+ and Propene Based on a DFT Study. *Organometallics*, **2006**, 25, 1643-1653	3.8	28
12	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
11	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
10	Migration of the subsurface C impurity in Pd(111). *Physical Review B*, **2005**, 71,	3.3	38
9	Composition Dependence of the Energy Barrier for Lithium Diffusion in Amorphous WO[sub 3]. *Electrochemical and Solid-State Letters*, **2005**, 8, J21		9
8	DFT Study of the Reaction between VO2+ and C2H6. *Organometallics*, **2004**, 23, 730-739	3.8	61
7	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
6	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
5	High-pressure behaviour of selenium-based spinels and related structures□n experimental and theoretical study. *Journal of Physics Condensed Matter*, **2004**, 16, 53-63	1.8	16
4	Bonding and compressibility in molecular and polymeric phases of solid CO2. *Journal of Physics Condensed Matter*, **2004**, 16, S1263-S1270	1.8	7
3	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
2	Quantum-mechanical simulation of MgAl2O4 under high pressure. *Physical Review B*, **2002**, 66,	3.3	37
1	Stability of MgAl 2 O 4 Under High-Pressure Conditions. *High Pressure Research*, **2002**, 22, 447-450	1.6	2