J AndrÃ©s

List of Publications by Year
in descending order

490	16,001	15466 65	46693 89
papers	citations	h-index	g-index

504	504	504	11865
all docs	docs citations	times ranked	citing authors

#	ARTICLE	IF	CITATIONS
1	A theoretical and experimental investigation of hetero- vs. homo-connectivity in barium silicates. American Mineralogist, 2022, 107, 716-728.	0.9	6
2	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.	2.7	2
3	Photoluminescence emissions of Ca1â^'WO4:xEu3+: Bridging between experiment and DFT calculations. Journal of Rare Earths, 2022, 40, 1527-1534.	2.5	6
4	Connecting morphology and photoluminescence emissions in Î²-Ag2MoO4 microcrystals. Ceramics International, 2022, 48, 3740-3750.	2.3	9
5	A diagnosis approach for semiconductor properties evaluation from ab initio calculations: Ag-based materials investigation. Journal of Solid State Chemistry, 2022, 305, 122670.	1.4	7
6	Tailoring Bi2MoO6 by Eu3+ incorporation for enhanced photoluminescence emissions. Journal of Luminescence, 2022, 243, 118675.	1.5	9
7	Graphene Nanoplatelets: In Vivo and In Vitro Toxicity, Cell Proliferative Activity, and Cell Gene Expression. Applied Sciences (Switzerland), 2022, 12, 720.	1.3	16
8	A bonding evolution theory study of the reaction between methylidyne radical, <scp>CH</scp>(<scp>X²Î</scp>), and cyclopentadiene, <scp>C₅H₆</scp>. International Journal of Quantum Chemistry, 2022, 122, .	1.0	6
9	Î± 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.	2.8	3
10	Interface matters: Design of an efficient Î±-Ag2WO4/Ag3PO4 photocatalyst. Materials Chemistry and Physics, 2022, 280, 125710.	2.0	7
11	Efficient Ni and Fe doping process in ZnO with enhanced photocatalytic activity: A theoretical and experimental investigation. Materials Research Bulletin, 2022, 152, 111849.	2.7	14
12	Inactivation of SARS-CoV-2 by a chitosan/Î±-Ag2WO4 composite generated by femtosecond laser irradiation. Scientific Reports, 2022, 12, 8118.	1.6	7
13	Formation of Metallic Ag on AgBr by Femtosecond Laser Irradiation. Physchem, 2022, 2, 179-190.	0.5	3
14	Towards a relationship between photoluminescence emissions and photocatalytic activity of Ag₂SeO₄: combining experimental data and theoretical insights. Dalton Transactions, 2022, 51, 11346-11362.	1.6	5
15	Deciphering the Molecular Mechanism of Intramolecular Reactions from the Perspective of Bonding Evolution Theory. Physchem, 2022, 2, 207-223.	0.5	4
16	Bridging experiment and theory: Morphology, optical, electronic, and magnetic properties of MnWO4. Applied Surface Science, 2022, 600, 154081.	3.1	9
17	Identifying and explaining vibrational modes of sanbornite (low-BaSi2O5) and Ba5Si8O21: A joint experimental and theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 248, 119130.	2.0	10
18	Modulating the properties of multifunctional semiconductors by means of morphology: Theory meets experiments. Computational Materials Science, 2021, 188, 110217.	1.4	19

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19	Revealing the Nature of Defects in Î±-Ag₂WO₄ by Positron Annihilation Lifetime Spectroscopy: A Joint Experimental and Theoretical Study. Crystal Growth and Design, 2021, 21, 1093-1102.	1.4	11
20	Unraveling a Biomass-Derived Multiphase Catalyst for the Dehydrogenative Coupling of Silanes with Alcohols under Aerobic Conditions. ACS Sustainable Chemistry and Engineering, 2021, 9, 2912-2928.	3.2	8
21	Structure, Photoluminescence Emissions, and Photocatalytic Activity of Ag₂SeO₃: A Joint Experimental and Theoretical Investigation. Inorganic Chemistry, 2021, 60, 5937-5954.	1.9	10
22	SiO2-Ag Composite as a Highly Virucidal Material: A Roadmap that Rapidly Eliminates SARS-CoV-2. Nanomaterials, 2021, 11, 638.	1.9	41
23	A scalable electron beam irradiation platform applied for allotropic carbon transformation. Carbon, 2021, 174, 567-580.	5.4	6
24	Surface-dependent photocatalytic and biological activities of Ag2CrO4: Integration of experiment and simulation. Applied Surface Science, 2021, 545, 148964.	3.1	18
25	PVC-SiO2-Ag composite as a powerful biocide and anti-SARS-CoV-2 material. Journal of Polymer Research, 2021, 28, 1.	1.2	15
26	Increasing the photocatalytic and fungicide activities of Ag3PO4 microcrystals under visible-light irradiation. Ceramics International, 2021, 47, 22604-22614.	2.3	13
27	Unveiling the Ag-Bi miscibility at the atomic level: A theoretical insight. Computational Materials Science, 2021, 197, 110612.	1.4	2
28	Carbon Nanofibers versus Silver Nanoparticles: Time-Dependent Cytotoxicity, Proliferation, and Gene Expression. Biomedicines, 2021, 9, 1155.	1.4	21
29	Bioactive Ag₃PO₄/Polypropylene Composites for Inactivation of SARS-CoV-2 and Other Important Public Health Pathogens. Journal of Physical Chemistry B, 2021, 125, 10866-10875.	1.2	10
30	Selective Synthesis of Î±-, Î²-, and Î³-Ag₂WO₄ Polymorphs: Promising Platforms for Photocatalytic and Antibacterial Materials. Inorganic Chemistry, 2021, 60, 1062-1079.	1.9	18
31	Catalytic Hydrogenation of Azobenzene in the Presence of a Cuboidal Mo₃S₄ Cluster via an Uncommon Sulfur-Based H₂ Activation Mechanism. ACS Catalysis, 2021, 11, 608-614.	5.5	22
32	Behavior of Bi2S3 under ultrasound irradiation for Rhodamine B dye degradation. Chemical Physics Letters, 2021, 785, 139123.	1.2	5
33	Protective Face Masks: Current Status and Future Trends. ACS Applied Materials & Interfaces, 2021, 13, 56725-56751.	4.0	76
34	Towards a white-emitting phosphor Ca10V6O25 based material. Journal of Luminescence, 2020, 220, 116990.	1.5	5
35	Structure, electronic properties, morphology evolution, and photocatalytic activity in PbMoO₄ and Pb_{1â^'2x}Ca_xSr_xMoO₄ (x = 0.1, 0.2, 0.3, 0.4 and 0.5) solid solutions. Physical Chemistry Chemical Physics, 2020, 22, 25876-25891.	1.3	12
36	Toward Expanding the Optical Response of Ag2CrO4 and Bi2O3 by Their Laser-Mediated Heterojunction. Journal of Physical Chemistry C, 2020, 124, 26404-26414.	1.5	2

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37	Structure, optical properties, and photocatalytic activity of Î±-Ag2W0.75Mo0.25O4. Materials Research Bulletin, 2020, 132, 111011.	2.7	8
38	Deciphering the Curly Arrow Representation and Electron Flow for the 1,3-Dipolar Rearrangement between Acetonitrile Oxide and (1S,2R,4S)-2-Cyano-7-oxabicyclo[2.2.1]hept-5-en-2-yl Acetate Derivatives. ACS Omega, 2020, 5, 22215-22225.	1.6	10
39	Rational Design of W-Doped Ag₃PO₄ as an Efficient Antibacterial Agent and Photocatalyst for Organic Pollutant Degradation. ACS Omega, 2020, 5, 23808-23821.	1.6	14
40	Unraveling the relationship between exposed surfaces and the photocatalytic activity of Ag₃PO₄: an in-depth theoretical investigation. RSC Advances, 2020, 10, 30640-30649.	1.7	12
41	Microwave-Driven Hexagonal-to-Monoclinic Transition in BiPO₄: An In-Depth Experimental Investigation and First-Principles Study. Inorganic Chemistry, 2020, 59, 7453-7468.	1.9	24
42	Surface-dependent properties of Î±-Ag2WO4: a joint experimental and theoretical investigation. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	19
43	Zinc-substituted Ag2CrO4: A material with enhanced photocatalytic and biological activity. Journal of Alloys and Compounds, 2020, 835, 155315.	2.8	16
44	Electron beam irradiation for the formation of thick Ag film on Ag₃PO₄. RSC Advances, 2020, 10, 21745-21753.	1.7	9
45	Metallic behavior in STO/LAO heterostructures with non-uniformly atomic interfaces. Materials Today Communications, 2020, 24, 101339.	0.9	1
46	Femtosecond-laser-irradiation-induced structural organization and crystallinity of Bi2WO6. Scientific Reports, 2020, 10, 4613.	1.6	9
47	A description of the formation and growth processes of CaTiO3 mesocrystals: a joint experimental and theoretical approach. Molecular Systems Design and Engineering, 2020, 5, 1255-1266.	1.7	5
48	The role of counter-ions in crystal morphology, surface structure and photocatalytic activity of ZnO crystals grown onto a substrate. Applied Surface Science, 2020, 529, 147057.	3.1	15
49	Unvealing the role of Î²-Ag2MoO4 microcrystals to the improvement of antibacterial activity. Materials Science and Engineering C, 2020, 111, 110765.	3.8	44
50	Connecting the surface structure, morphology and photocatalytic activity of Ag2O: An in depth and unified theoretical investigation. Applied Surface Science, 2020, 509, 145321.	3.1	51
51	Ag Nanoparticles/AgX (X=Cl, Br and I) Composites with Enhanced Photocatalytic Activity and Low Toxicological Effects. ChemistrySelect, 2020, 5, 4655-4673.	0.7	29
52	Unconventional Magnetization Generated from Electron Beam and Femtosecond Irradiation on Î±-Ag₂WO₄: A Quantum Chemical Investigation. ACS Omega, 2020, 5, 10052-10067.	1.6	20
53	Geometry, electronic structure, morphology, and photoluminescence emissions of BaW1-xMoxO4 (xâ€¯=â€¯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
54	Computational procedure to an accurate DFT simulation to solid state systems. Computational Materials Science, 2019, 170, 109176.	1.4	17

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55	Joint Theoretical and Experimental Study on the La Doping Process in In₂O₃: Phase Transition and Electrocatalytic Activity. Inorganic Chemistry, 2019, 58, 11738-11750.	1.9	22
56	On the catalytic transfer hydrogenation of nitroarenes by a cubane-type Mo₃S₄ cluster hydride: disentangling the nature of the reaction mechanism. Physical Chemistry Chemical Physics, 2019, 21, 17221-17231.	1.3	6
57	Ag Nanoparticles/Î±-Ag2WO4 Composite Formed by Electron Beam and Femtosecond Irradiation as Potent Antifungal and Antitumor Agents. Scientific Reports, 2019, 9, 9927.	1.6	40
58	Evidence for the formation of metallic In after laser irradiation of InP. Journal of Applied Physics, 2019, 126, .	1.1	4
59	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.	1.5	45
60	Nine questions on energy decomposition analysis. Journal of Computational Chemistry, 2019, 40, 2248-2283.	1.5	113
61	Unveiling the efficiency of microwave-assisted hydrothermal treatment for the preparation of SrTiO₃ mesocrystals. Physical Chemistry Chemical Physics, 2019, 21, 22031-22038.	1.3	11
62	In Situ Growth of Bi Nanoparticles on NaBiO₃, Î´-, and Î²-Bi₂O₃ Surfaces: Electron Irradiation and Theoretical Insights. Journal of Physical Chemistry C, 2019, 123, 5023-5030.	1.5	14
63	How effectively bonding evolution theory retrieves and visualizes curly arrows: The cycloaddition reaction of cyclic nitrones. International Journal of Quantum Chemistry, 2019, 119, e25985.	1.0	18
64	Î±-AgVO₃ Decorated by Hydroxyapatite (Ca₁₀(PO₄)₆(OH)₂): Tuning Its Photoluminescence Emissions and Bactericidal Activity. Inorganic Chemistry, 2019, 58, 5900-5913.	1.9	22
65	Proofâ€ofâ€Concept Studies Directed toward the Formation of Metallic Ag Nanostructures from Ag 3 PO 4 Induced by Electron Beam and Femtosecond Laser. Particle and Particle Systems Characterization, 2019, 36, 1800533.	1.2	10
66	Connecting Theory with Experiment to Understand the Sintering Processes of Ag Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 11310-11318.	1.5	16
67	Laser and electron beam-induced formation of Ag/Cr structures on Ag₂CrO₄. Physical Chemistry Chemical Physics, 2019, 21, 6101-6111.	1.3	20
68	Designing biocompatible and multicolor fluorescent hydroxyapatite nanoparticles for cell-imaging applications. Materials Today Chemistry, 2019, 14, 100211.	1.7	14
69	Palladium doping of In₂O₃ towards a general and selective catalytic hydrogenation of amides to amines and alcohols. Catalysis Science and Technology, 2019, 9, 6965-6976.	2.1	19
70	First principle investigation of the exposed surfaces and morphology of Î²-ZnMoO4. Journal of Applied Physics, 2019, 126, 235301.	1.1	14
71	Polymorphs of ZnV₂O₆ under Pressure: A First-Principle Investigation. Journal of Physical Chemistry C, 2019, 123, 3239-3253.	1.5	16
72	Tailoring the Bactericidal Activity of Ag Nanoparticles/Î±-Ag₂WO₄ Composite Induced by Electron Beam and Femtosecond Laser Irradiation: Integration of Experiment and Computational Modeling. ACS Applied Bio Materials, 2019, 2, 824-837.	2.3	30

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73	Towards enhancing the magnetic properties by morphology control of ATiO3 (Aâ€¯=â€¯Mn, Fe, Ni) multiferroic materials. Journal of Magnetism and Magnetic Materials, 2019, 475, 544-549.	1.0	29
74	Structure, morphology and photoluminescence emissions of ZnMoO4: RE 3+=Tb3+ - Tm3+ - X Eu3+ (xÂ= 1,) Tj ETQq0 0 0 rgBT /Overloc Compounds, 2018, 750, 55-70.	2.8	34
75	Laser-induced formation of bismuth nanoparticles. Physical Chemistry Chemical Physics, 2018, 20, 13693-13696.	1.3	17
76	Towards the scale-up of the formation of nanoparticles on Î±-Ag2WO4 with bactericidal properties by femtosecond laser irradiation. Scientific Reports, 2018, 8, 1884.	1.6	42
77	Can Supported Reduced Vanadium Oxides form H₂ from CH₃OH? A Computational Gas-Phase Mechanistic Study. Journal of Physical Chemistry A, 2018, 122, 1104-1113.	1.1	7
78	ZnWO₄ nanocrystals: synthesis, morphology, photoluminescence and photocatalytic properties. Physical Chemistry Chemical Physics, 2018, 20, 1923-1937.	1.3	103
79	Î±- and Î²-AgVO3 polymorphs as photoluminescent materials: An example of temperature-driven synthesis. Ceramics International, 2018, 44, 5939-5944.	2.3	21
80	Binding free energy calculations to rationalize the interactions of huprines with acetylcholinesterase. Journal of Computer-Aided Molecular Design, 2018, 32, 607-622.	1.3	2
81	Improving the ozone gas-sensing properties of CuWO4 nanoparticles. Journal of Alloys and Compounds, 2018, 748, 411-417.	2.8	44
82	Surfactant-Mediated Morphology and Photocatalytic Activity of Î±-Ag₂WO₄ Material. Journal of Physical Chemistry C, 2018, 122, 8667-8679.	1.5	60
83	Structural properties and self-activated photoluminescence emissions in hydroxyapatite with distinct particle shapes. Ceramics International, 2018, 44, 236-245.	2.3	36
84	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
85	Formation of Ag nanoparticles under electron beam irradiation: Atomistic origins from firstâ€principles calculations. International Journal of Quantum Chemistry, 2018, 118, e25551.	1.0	21
86	A bonding evolution analysis for the thermal Claisen rearrangement: an experimental and theoretical exercise for testing the electron density flow. Physical Chemistry Chemical Physics, 2018, 20, 535-541.	1.3	13
87	Theoretical approach for determining the relation between the morphology and surface magnetism of Co3O4. Journal of Magnetism and Magnetic Materials, 2018, 453, 262-267.	1.0	42
88	Computational Chemistry Meets Experiments for Explaining the Geometry, Electronic Structure, and Optical Properties of Ca₁₀V₆O₂₅. Inorganic Chemistry, 2018, 57, 15489-15499.	1.9	18
89	Direct preparation of standard functional interfaces in oxide heterostructures for 2DEG analysis through beam-induced platinum contacts. Applied Physics Letters, 2018, 113, .	1.5	2
90	In situ Formation of Metal Nanoparticles through Electron Beam Irradiation: Modeling Real Materials from First-Principles Calculations. Journal of Material Science & Engineering, 2018, 07, .	0.2	8

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91	Laser/Electron Irradiation on Indium Phosphide (InP) Semiconductor: Promising Pathways to In Situ Formation of Indium Nanoparticles. Particle and Particle Systems Characterization, 2018, 35, 1800237.	1.2	12
92	A DFT investigation of the role of oxygen vacancies on the structural, electronic and magnetic properties of ATiO₃ (A = Mn, Fe, Ni) multiferroic materials. Physical Chemistry Chemical Physics, 2018, 20, 28382-28392.	1.3	26
93	Cuboidal Mo₃S₄ Clusters as a Platform for Exploring Catalysis: A Three-Center Sulfur Mechanism for Alkyne Semihydrogenation. ACS Catalysis, 2018, 8, 7346-7350.	5.5	12
94	Connecting structural, optical, and electronic properties and photocatalytic activity of Ag3PO4:Mo complemented by DFT calculations. Applied Catalysis B: Environmental, 2018, 238, 198-211.	10.8	53
95	Magnetism and multiferroic properties at MnTiO3 surfaces: A DFT study. Applied Surface Science, 2018, 452, 463-472.	3.1	45
96	Chemical Bond Formation and Rupture Processes: An Application of DFTâ€“Chemical Pressure Approach. Journal of Physical Chemistry C, 2018, 122, 21216-21225.	1.5	9
97	From Complex Inorganic Oxides to Agâ€“Bi Nanoalloy: Synthesis by Femtosecond Laser Irradiation. ACS Omega, 2018, 3, 9880-9887.	1.6	19
98	Experimental and theoretical study of the energetic, morphological, and photoluminescence properties of CaZrO₃:Eu³⁺. CrystEngComm, 2018, 20, 5519-5530.	1.3	22
99	Computational Modeling for the Ag Nanoparticle Coalescence Process: A Case of Surface Plasmon Resonance. Journal of Physical Chemistry C, 2017, 121, 7030-7036.	1.5	16
100	Synthesis and evaluation of Î±-Ag2WO4 as novel antifungal agent. Chemical Physics Letters, 2017, 674, 125-129.	1.2	30
101	Synthesis of Cuboctahedral CeO₂ Nanoclusters and Their Assembly into Cuboid Nanoparticles by Oriented Attachment. ChemNanoMat, 2017, 3, 228-232.	1.5	10
102	The interplay between morphology and photocatalytic activity in ZnO and N-doped ZnO crystals. Materials and Design, 2017, 120, 363-375.	3.3	79
103	Binding Analysis of Some Classical Acetylcholinesterase Inhibitors: Insights for a Rational Design Using Free Energy Perturbation Method Calculations with QM/MM MD Simulations. Journal of Chemical Information and Modeling, 2017, 57, 958-976.	2.5	28
104	Electronic structure and rearrangements of anionic [ClMg(Î·2-O2C)]â^' and [ClMg(Î·2-CO2)]â^' complexes: a quantum chemical topology study. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	8
105	On the outside looking in: rethinking the molecular mechanism of 1,3-dipolar cycloadditions from the perspective of bonding evolution theory. The reaction between cyclic nitrones and ethyl acrylate. Physical Chemistry Chemical Physics, 2017, 19, 18288-18302.	1.3	31
106	Î±-Ag_{2â€“2x}Zn_xWO₄ (0 â‰¤ x â‰¤ 0.25) Solid Solutions: Structure, Morphology, and Optical Properties. Inorganic Chemistry, 2017, 56, 7360-7372.	1.9	36
107	Mechanism of Antibacterial Activity via Morphology Change of Î±-AgVO₃: Theoretical and Experimental Insights. ACS Applied Materials & Interfaces, 2017, 9, 11472-11481.	4.0	53
108	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.	1.9	46

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109	A novel approach to obtain highly intense self-activated photoluminescence emissions in hydroxyapatite nanoparticles. Journal of Solid State Chemistry, 2017, 249, 64-69.	1.4	24
110	Curly arrows, electron flow, and reaction mechanisms from the perspective of the bonding evolution theory. Physical Chemistry Chemical Physics, 2017, 19, 29031-29046.	1.3	36
111	Tuning the Morphological, Optical, and Antimicrobial Properties of Î±-Ag₂WO₄ Microcrystals Using Different Solvents. Crystal Growth and Design, 2017, 17, 6239-6246.	1.4	35
112	First-Principles Study on Polymorphs of AgVO₃: Assessing to Structural Stabilities and Pressure-Induced Transitions. Journal of Physical Chemistry C, 2017, 121, 27624-27642.	1.5	22
113	Bridging Structure and Real-Space Topology: Understanding Complex Molecules and Solid-State Materials. , 2017, , 427-454.		2
114	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.	2.8	16
115	Uncovering the metastable Î³-Ag₂WO₄phase: a joint experimental and theoretical study. RSC Advances, 2017, 7, 5610-5620.	1.7	22
116	Photoluminescent properties of ZrO2: Tm3+, Tb3+, Eu3+ powdersâ€"A combined experimental and theoretical study. Journal of Alloys and Compounds, 2017, 695, 3094-3103.	2.8	50
117	Disclosing the electronic structure and optical properties of Ag₄V₂O₇crystals: experimental and theoretical insights. CrystEngComm, 2016, 18, 6483-6491.	1.3	15
118	Effects of chemical substitution on the structural and optical properties of Î±-Ag_{2âˆ'2x}Ni_xWO₄(0 â‰¤ x â‰¤ 0.08) solid solutions. Physical Chemistry Chemical Physics, 2016, 18, 21966-21975.	1.3	24
119	An Experimental and Computational Study of Î²-AgVO₃: Optical Properties and Formation of Ag Nanoparticles. Journal of Physical Chemistry C, 2016, 120, 12254-12264.	1.5	48
120	In situgrowth of Ag nanoparticles onÎ±-Ag₂WO₄under electron irradiation: probing the physical principles. Nanotechnology, 2016, 27, 225703.	1.3	30
121	Curly arrows meet electron density transfers in chemical reaction mechanisms: from electron localization function (ELF) analysis to valence-shell electron-pair repulsion (VSEPR) inspired interpretation. Chemical Communications, 2016, 52, 8183-8195.	2.2	66
122	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.	1.4	27
123	Synthesis and morphological transformation of BaWO4 crystals: Experimental and theoretical insights. Ceramics International, 2016, 42, 10913-10921.	2.3	45
124	Acetone gas sensor based on Î±-Ag2WO4 nanorods obtained via a microwave-assisted hydrothermal route. Journal of Alloys and Compounds, 2016, 683, 186-190.	2.8	66
125	On the morphology of BaMoO₄ crystals: A theoretical and experimental approach. Crystal Research and Technology, 2016, 51, 634-644.	0.6	24
126	Modeling the atomic-scale structure, stability, and morphological transformations in the tetragonal phase of LaVO4. Chemical Physics Letters, 2016, 660, 87-92.	1.2	34

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127	Theoretical and Experimental Insight on Ag₂CrO₄ Microcrystals: Synthesis, Characterization, and Photoluminescence Properties. Inorganic Chemistry, 2016, 55, 8961-8970.	1.9	31
128	Formation of Ag Nanoparticles on Î²-Ag₂WO₄ through Electron Beam Irradiation: A Synergetic Computational and Experimental Study. Inorganic Chemistry, 2016, 55, 8661-8671.	1.9	38
129	In situ Transmission Electron Microscopy observation of Ag nanocrystal evolution by surfactant free electron-driven synthesis. Scientific Reports, 2016, 6, 21498.	1.6	41
130	Photoluminescence and Photocatalytic Properties of Ag₃PO₄ Microcrystals: An Experimental and Theoretical Investigation. ChemPlusChem, 2016, 81, 202-212.	1.3	70
131	Synthesis, antifungal evaluation and optical properties of silver molybdate microcrystals in different solvents: a combined experimental and theoretical study. Dalton Transactions, 2016, 45, 10736-10743.	1.6	49
132	A numerical simulation of woven/anionic polyamide 6 composite part manufacturing using structural reactive injection moulding process. Journal of Thermoplastic Composite Materials, 2016, 29, 219-233.	2.6	5
133	Formation of Ag nanoparticles on metastable Î²-Ag2WO4 microcrystals induced by electron irradiation. Chemical Physics Letters, 2016, 644, 68-72.	1.2	31
134	A 3D platform for the morphology modulation of materials: first principles calculations on the thermodynamic stability and surface structure of metal oxides: Co₃O₄,Î±-Fe₂O₃, and In₂O₃. Modelling and Simulation in Materials Science and Engineering, 2016, 24, 025007.	0.8	53
135	Synthesis and characterization of metastable Î²-Ag₂WO₄: an experimental and theoretical approach. Dalton Transactions, 2016, 45, 1185-1191.	1.6	24
136	Quantum Chemical Topology Approach for Dissecting Chemical Structure and Reactivity. Challenges and Advances in Computational Chemistry and Physics, 2016, , 257-294.	0.6	2
137	Chemical Bonding under Pressure. , 2015, , 131-157.		0
138	A Combined Experimental and Theoretical Study on the Formation of Ag Filaments on Î²â€Ag₂MoO₄ Induced by Electron Irradiation. Particle and Particle Systems Characterization, 2015, 32, 646-651.	1.2	47
139	Effects of surface stability on the morphological transformation of metals and metal oxides as investigated by first-principles calculations. Nanotechnology, 2015, 26, 405703.	1.3	84
140	Facet-dependent photocatalytic and antibacterial properties of Î±-Ag₂WO₄crystals: combining experimental data and theoretical insights. Catalysis Science and Technology, 2015, 5, 4091-4107.	2.1	123
141	Elucidating the real-time Ag nanoparticle growth on Î±-Ag₂WO₄during electron beam irradiation: experimental evidence and theoretical insights. Physical Chemistry Chemical Physics, 2015, 17, 5352-5359.	1.3	54
142	Identifying and rationalizing the morphological, structural, and optical properties of Î²-Ag₂MoO₄ 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.	2.8	61
143	Inquiry of the electron density transfers in chemical reactions: a complete reaction path for the denitrogenation process of 2,3-diazabicyclo[2.2.1]hept-2-ene derivatives. Physical Chemistry Chemical Physics, 2015, 17, 32358-32374.	1.3	10
144	Structural and optical properties of ZnS/MgNb2O6 heterostructures. Superlattices and Microstructures, 2015, 79, 180-192.	1.4	6

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145	A relationship between structural and electronic orderâ€“disorder effects and optical properties in crystalline TiO₂nanomaterials. Dalton Transactions, 2015, 44, 3159-3175.	1.6	96
146	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.	1.8	22
147	Joint Use of Bonding Evolution Theory and QM/MM Hybrid Method for Understanding the Hydrogen Abstraction Mechanism via Cytochrome P450 Aromatase. Journal of Chemical Theory and Computation, 2015, 11, 1470-1480.	2.3	17
148	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.	1.5	120
149	Fingerprints of short-range and long-range structure in BaZr_{1â”’x}Hf_xO₃ solid solutions: an experimental and theoretical study. Physical Chemistry Chemical Physics, 2015, 17, 11341-11349.	1.3	10
150	Quantum chemical topological analysis of hydrogen bonding in HXâ€¦HX and CH₃Xâ€¦HX dimers (XÂ=Â Br, Cl, F). Molecular Simulation, 2015, 41, 600-609.	0.9	8
151	Chemical structure and reactivity by means of quantum chemical topology analysis. Computational and Theoretical Chemistry, 2015, 1053, 17-30.	1.1	62
152	Silver Molybdate and Silver Tungstate Nanocomposites with Enhanced Photoluminescence. Nanomaterials and Nanotechnology, 2014, 4, 22.	1.2	83
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