J AndrÃ©s

List of Publications by Year
in descending order

490 papers	16,001 citations	15504 65 h-index	46799 89 g-index
504 all docs	504 docs citations	504 times ranked	11865 citing authors

#	ARTICLE	IF	CITATIONS
1	Crystal growth in colloidal tin oxide nanocrystals induced by coalescence at room temperature. Applied Physics Letters, 2003, 83, 1566-1568.	3.3	257
2	Structural and optical properties of CaTiO3 perovskite-based materials obtained by microwave-assisted hydrothermal synthesis: An experimental and theoretical insight. Acta Materialia, 2009, 57, 5174-5185.	7.9	194
3	Morphology and Blue Photoluminescence Emission of PbMoO₄ Processed in Conventional Hydrothermal. Journal of Physical Chemistry C, 2009, 113, 5812-5822.	3.1	171
4	Understanding Reaction Mechanisms in Organic Chemistry from Catastrophe Theory Applied to the Electron Localization Function Topology. Journal of Physical Chemistry A, 2008, 112, 7128-7136.	2.5	165
5	An Aromaticity Scale Based on the Topological Analysis of the Electron Localization Function Including Ïƒ and Ï€ Contributions. Journal of Chemical Theory and Computation, 2005, 1, 83-86.	5.3	152
6	Theoretical insights in enzyme catalysis. Chemical Society Reviews, 2004, 33, 98-107.	38.1	150
7	Electronic structure and optical properties of BaMoO4 powders. Current Applied Physics, 2010, 10, 614-624.	2.4	150
8	The Joint Use of Catastrophe Theory and Electron Localization Function to Characterize Molecular Mechanisms. A Density Functional Study of the Dielsâ^'Alder Reaction between Ethylene and 1,3-Butadiene. Journal of Physical Chemistry A, 2003, 107, 6014-6024.	2.5	149
9	Influence of Reactant Polarity on the Course of the Inverse-Electron-Demand Dielsâ^'Alder Reaction. A DFT Study of Regio- and Stereoselectivity, Presence of Lewis Acid Catalyst, and Inclusion of Solvent Effects in the Reaction between Nitroethene and Substituted Ethenes. Journal of Organic Chemistry, 1999, 64, 5867-5875.	3.2	136
10	Hierarchical Assembly of CaMoO₄ Nano-Octahedrons and Their Photoluminescence Properties. Journal of Physical Chemistry C, 2011, 115, 5207-5219.	3.1	130
11	New Findings on the Dielsâ^'Alder Reactions. An Analysis Based on the Bonding Evolution Theory. Journal of Physical Chemistry A, 2006, 110, 13939-13947.	2.5	128
12	Toward an Understanding of the Growth of Ag Filaments on Î±-Ag₂WO₄ and Their Photoluminescent Properties: A Combined Experimental and Theoretical Study. Journal of Physical Chemistry C, 2014, 118, 1229-1239.	3.1	124
13	Facet-dependent photocatalytic and antibacterial properties of Î±-Ag₂WO₄crystals: combining experimental data and theoretical insights. Catalysis Science and Technology, 2015, 5, 4091-4107.	4.1	123
14	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.	3.1	120
15	Density Functional Theory Study of the Brookite Surfaces and Phase Transitions between Natural Titania Polymorphs. Journal of Physical Chemistry B, 2006, 110, 23417-23423.	2.6	119
16	Static simulation of bulk and selected surfaces of anatase TiO2. Surface Science, 2001, 490, 116-124.	1.9	115
17	Thermodynamic argument about SnO2 nanoribbon growth. Applied Physics Letters, 2003, 83, 635-637.	3.3	115
18	Nine questions on energy decomposition analysis. Journal of Computational Chemistry, 2019, 40, 2248-2283.	3.3	113

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19	Efficient microwave-assisted hydrothermal synthesis of CuO sea urchin-like architectures via a mesoscale self-assembly. CrystEngComm, 2010, 12, 1696.	2.6	109
20	A Systematic Density Functional Theory Study of VxOy+ and VxOY (X = 2â^'4, Y = 2â^'10) Systems. Journal of Physical Chemistry A, 2001, 105, 9760-9775.	2.5	107
21	Synthesis of wurtzite ZnS nanoparticles using the microwave assisted solvothermal method. Journal of Alloys and Compounds, 2013, 556, 153-159.	5.5	105
22	A novel ozone gas sensor based on one-dimensional (1D) Î±-Ag₂WO₄ nanostructures. Nanoscale, 2014, 6, 4058-4062.	5.6	105
23	Room-temperature photoluminescence ofBaTiO3:â€ƒJoint experimental and theoretical study. Physical Review B, 2005, 71, .	3.2	103
24	Direct in situ observation of the electron-driven synthesis of Ag filaments on Î±-Ag2WO4 crystals. Scientific Reports, 2013, 3, 1676.	3.3	103
25	ZnWO₄ nanocrystals: synthesis, morphology, photoluminescence and photocatalytic properties. Physical Chemistry Chemical Physics, 2018, 20, 1923-1937.	2.8	103
26	Periodic study on the structural and electronic properties of bulk, oxidized and reduced SnO 2 (1 1 0) surfaces and the interaction with O 2. Surface Science, 2002, 511, 408-420.	1.9	100
27	A Theoretical Study on the Relationship between Nucleophilicity and Ionization Potentials in Solution Phase. Journal of Physical Chemistry A, 2003, 107, 5588-5593.	2.5	100
28	Zinc blende versus wurtzite ZnS nanoparticles: control of the phase and optical properties by tetrabutylammonium hydroxide. Physical Chemistry Chemical Physics, 2014, 16, 20127-20137.	2.8	100
29	Potentiated Electron Transference in Î±-Ag₂WO₄ Microcrystals with Ag Nanofilaments as Microbial Agent. Journal of Physical Chemistry A, 2014, 118, 5769-5778.	2.5	99
30	Structural and electronic analysis of the atomic scale nucleation of Ag on Î±-Ag2WO4 induced by electron irradiation. Scientific Reports, 2014, 4, 5391.	3.3	99
31	Density functional theory calculation of the electronic structure ofBa0.5Sr0.5TiO3:Photoluminescent properties and structural disorder. Physical Review B, 2004, 69, .	3.2	98
32	A relationship between structural and electronic orderâ€“disorder effects and optical properties in crystalline TiO₂nanomaterials. Dalton Transactions, 2015, 44, 3159-3175.	3.3	96
33	Understanding the Molecular Mechanism of the 1,3-Dipolar Cycloaddition between Fulminic Acid and Acetylene in Terms of the Electron Localization Function and Catastrophe Theory. Chemistry - A European Journal, 2004, 10, 5165-5172.	3.3	95
34	A Hybrid Potential Reaction Path and Free Energy Study of the Chorismate Mutase Reaction. Journal of the American Chemical Society, 2001, 123, 1709-1712.	13.7	92
35	Enhancing Reactivity of Carbonyl Compounds via Hydrogen-Bond Formation. A DFT Study of the Hetero-Dielsâ^'Alder Reaction between Butadiene Derivative and Acetone in Chloroform. Journal of Organic Chemistry, 2003, 68, 8662-8668.	3.2	91
36	Long-range and short-range structures of cube-like shape SrTiO3 powders: microwave-assisted hydrothermal synthesis and photocatalytic activity. Physical Chemistry Chemical Physics, 2013, 15, 12386.	2.8	91

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37	Synthesis of Fine Micro-sized BaZrO₃ Powders Based on a Decaoctahedron Shape by the Microwave-Assisted Hydrothermal Method. Crystal Growth and Design, 2009, 9, 833-839.	3.0	86
38	Presence of excited electronic state in CaWO4 crystals provoked by a tetrahedral distortion: An experimental and theoretical investigation. Journal of Applied Physics, 2011, 110, .	2.5	84
39	Unraveling reaction mechanisms by means of Quantum Chemical Topology Analysis. International Journal of Quantum Chemistry, 2014, 114, 1239-1252.	2.0	84
40	Effects of surface stability on the morphological transformation of metals and metal oxides as investigated by first-principles calculations. Nanotechnology, 2015, 26, 405703.	2.6	84
41	A combined theoretical and experimental study of electronic structure and optical properties of Î²-ZnMoO4 microcrystals. Polyhedron, 2013, 54, 13-25.	2.2	83
42	Silver Molybdate and Silver Tungstate Nanocomposites with Enhanced Photoluminescence. Nanomaterials and Nanotechnology, 2014, 4, 22.	3.0	83
43	Characterization of the High-Pressure Structures and Phase Transformations in SnO2. A Density Functional Theory Study. Journal of Physical Chemistry B, 2007, 111, 6479-6485.	2.6	82
44	Theoretical Modeling of Enzyme Catalytic Power:Â Analysis of â€œCraticâ€•and Electrostatic Factors in CatecholO-Methyltransferase. Journal of the American Chemical Society, 2003, 125, 7726-7737.	13.7	79
45	Describing the Molecular Mechanism of Organic Reactions by Using Topological Analysis of Electronic Localization Function. Current Organic Chemistry, 2011, 15, 3566-3575.	1.6	79
46	The interplay between morphology and photocatalytic activity in ZnO and N-doped ZnO crystals. Materials and Design, 2017, 120, 363-375.	7.0	79
47	Catalytic Mechanism of Dihydrofolate Reductase Enzyme. A Combined Quantum-Mechanical/Molecular-Mechanical Characterization of Transition State Structure for the Hydride Transfer Step. Journal of the American Chemical Society, 1999, 121, 12140-12147.	13.7	78
48	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.	3.1	76
49	Protective Face Masks: Current Status and Future Trends. ACS Applied Materials & Interfaces, 2021, 13, 56725-56751.	8.0	76
50	Structure and Bonding of Chlorine Oxides and Peroxides:Â ClOx, ClOx-(x= 1â^'4), and Cl2Ox(x= 1â^'8). Journal of Physical Chemistry A, 1999, 103, 3078-3088.	2.5	74
51	A simple protocol to help calculate saddle points. Transition-state structures for the Meyerâ€"Schuster reaction in non-aqueous media: An ab initio MO study. Chemical Physics Letters, 1984, 109, 471-477.	2.6	73
52	A Joint Experimental and Theoretical Study on the Nanomorphology of CaWO₄ Crystals. Journal of Physical Chemistry C, 2011, 115, 20113-20119.	3.1	73
53	A theoretical study on the structure, energetics and bonding of VOx+ and VOx (x=1â€"4) systems. Chemical Physics Letters, 2001, 333, 493-503.	2.6	72
54	An efficient microwave-assisted hydrothermal synthesis of BaZrO3 microcrystals: growth mechanism and photoluminescence emissions. CrystEngComm, 2010, 12, 3612.	2.6	72

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55	Topological Analysis of Multiple Metalâ^'Metal Bonds in Dimers of the M2(Formamidinate)4Type with M = Nb, Mo, Tc, Ru, Rh, and Pd. Journal of Physical Chemistry A, 2001, 105, 9460-9466.	2.5	71
56	Electronic and structural properties of SnxTi1â^'xO2 solid solutions: a periodic DFT study. Catalysis Today, 2003, 85, 145-152.	4.4	71
57	A theoretical analysis of adsorption and dissociation of CH3OH on the stoichiometric SnO2(110) surface. Surface Science, 1999, 430, 213-222.	1.9	70
58	Photoluminescence and Photocatalytic Properties of Ag₃PO₄ Microcrystals: An Experimental and Theoretical Investigation. ChemPlusChem, 2016, 81, 202-212.	2.8	70
59	First principles calculations on the origin of violet-blue and green light photoluminescence emission in SrZrO3 and SrTiO3 perovskites. Theoretical Chemistry Accounts, 2009, 124, 385-394.	1.4	69
60	An improved method for preparation of SrTiO3 nanoparticles. Materials Chemistry and Physics, 2011, 125, 168-173.	4.0	69
61	Transition structure for hydride transfer to pyridinium cation from methanolate. Modeling of LADH catalyzed reaction. Journal of the American Chemical Society, 1988, 110, 4046-4047.	13.7	68
62	Quantum-mechanical analysis of the equation of state of anataseTiO2. Physical Review B, 2001, 64, .	3.2	68
63	Theoretical Study on the Molecular Mechanism for the Reaction of VO2+ with C2H4. Journal of Physical Chemistry A, 2003, 107, 3107-3120.	2.5	68
64	On the photoluminescence behavior of samarium-doped strontium titanate nanostructures under UV light. A structural and electronic understanding. Physical Chemistry Chemical Physics, 2010, 12, 7566.	2.8	68
65	A theoretical study of the Meyer-Schuster reaction mechanism: minimum-energy profile and properties of transition-state structure. Journal of the American Chemical Society, 1988, 110, 666-674.	13.7	67
66	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.	4.1	66
67	Acetone gas sensor based on Î±-Ag2WO4 nanorods obtained via a microwave-assisted hydrothermal route. Journal of Alloys and Compounds, 2016, 683, 186-190.	5.5	66
68	Density Functional Theory Study on the Structural and Electronic Properties of Low Index Rutile Surfaces for TiO₂/SnO₂/TiO₂ and SnO₂/TiO₂/SnO₂ Composite Systems. Journal of Physical Chemistry A, 2008, 112, 8943-8952.	2.5	65
69	The hierarchy of localization basins: a tool for the understanding of chemical bonding exemplified by the analysis of the VO x and VO x + (x =1-4) systems. Theoretical Chemistry Accounts, 2001, 105, 299-308.	1.4	64
70	Toward an Understanding of Intermediate- and Short-Range Defects in ZnO Single Crystals. A Combined Experimental and Theoretical Study. Journal of Physical Chemistry A, 2008, 112, 8970-8978.	2.5	64
71	Structural refinement, growth mechanism, infrared/Raman spectroscopies and photoluminescence properties of PbMoO4 crystals. Polyhedron, 2013, 50, 532-545.	2.2	63
72	Quantum Mechanics Insight into the Microwave Nucleation of SrTiO₃ Nanospheres. Journal of Physical Chemistry C, 2012, 116, 24792-24808.	3.1	62

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73	Chemical structure and reactivity by means of quantum chemical topology analysis. Computational and Theoretical Chemistry, 2015, 1053, 17-30.	2.5	62
74	A theoretical study on cytosine tautomers in aqueous media by using continuum models. Chemical Physics Letters, 2000, 317, 437-443.	2.6	61
75	DFT Study of the Reaction between VO2+ and C2H6. Organometallics, 2004, 23, 730-739.	2.3	61
76	Unveiling the Chemical and Morphological Features of Sbâ^'SnO₂ Nanocrystals by the Combined Use of High-Resolution Transmission Electron Microscopy and ab Initio Surface Energy Calculations. Journal of the American Chemical Society, 2009, 131, 14544-14548.	13.7	61
77	Following the Molecular Mechanism for the NH₃ + LiH â†' LiNH₂ + H₂ Chemical Reaction: A Study Based on the Joint Use of the Quantum Theory of Atoms in Molecules (QTAIM) and Noncovalent Interaction (NCI) Index. Journal of Physical Chemistry A, 2014, 118, 1663-1672.	2.5	61
78	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.	6.1	61
79	Toward an Understanding of Molecular Mechanism of Domino Cycloadditions. Density Functional Theory Study of the Reaction between Hexafluorobut-2-yne andN,Nâ€˜-Dipyrrolylmethane. Journal of the American Chemical Society, 1998, 120, 1617-1618.	13.7	60
80	Origin of photoluminescence in SrTiO3: a combined experimental and theoretical study. Journal of Solid State Chemistry, 2004, 177, 3879-3885.	2.9	60
81	Towards understanding of magnetic interactions within a series of tetrathiafulvaleneâ€“Ï€ conjugated-verdazyl diradical cation system: a density functional theory study. Physical Chemistry Chemical Physics, 2008, 10, 857-864.	2.8	60
82	Surfactant-Mediated Morphology and Photocatalytic Activity of Î±-Ag₂WO₄ Material. Journal of Physical Chemistry C, 2018, 122, 8667-8679.	3.1	60
83	Nucleophilicity Index from Perturbed Electrostatic Potentials. Journal of Physical Chemistry A, 2007, 111, 2442-2447.	2.5	59
84	Preorganization and Reorganization as Related Factors in Enzyme Catalysis: The Chorismate Mutase Case. Chemistry - A European Journal, 2003, 9, 984-991.	3.3	57
85	A Theoretical Study on the Reaction Mechanism for the Bergman Cyclization from the Perspective of the Electron Localization Function and Catastrophe Theory. Journal of Physical Chemistry A, 2005, 109, 3687-3693.	2.5	57
86	A joint study based on the electron localization function and catastrophe theory of the chameleonic and centauric models for the Cope rearrangement of 1,5-hexadiene and its cyano derivatives. Journal of Computational Chemistry, 2005, 26, 1427-1437.	3.3	56
87	First-Principles Study of Pressure-Induced Phase Transitions and Electronic Properties of Ag₂MoO₄. Journal of Physical Chemistry C, 2014, 118, 3724-3732.	3.1	56
88	A QM/MM Study of the Conformational Equilibria in the Chorismate Mutase Active Site. The Role of the Enzymatic Deformation Energy Contribution. Journal of Physical Chemistry B, 2000, 104, 11308-11315.	2.6	54
89	An electron localization function study of the trimerization of acetylene: Reaction mechanism and development of aromaticity. Chemical Physics Letters, 2005, 406, 393-397.	2.6	54
90	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.	2.8	54

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91	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.	2.0	53
92	Mechanism of Antibacterial Activity via Morphology Change of Î±-AgVO₃: Theoretical and Experimental Insights. ACS Applied Materials & Interfaces, 2017, 9, 11472-11481.	8.0	53
93	Connecting structural, optical, and electronic properties and photocatalytic activity of Ag3PO4:Mo complemented by DFT calculations. Applied Catalysis B: Environmental, 2018, 238, 198-211.	20.2	53
94	Lithium insertion and mobility in the TiO2-anatase/titanate structure: A periodic DFT study. Journal of Electroanalytical Chemistry, 2005, 581, 216-223.	3.8	52
95	Theoretical Study of the Gas Phase Decomposition of Glycolic, Lactic, and 2-Hydroxyisobutyric Acids. Journal of the American Chemical Society, 1997, 119, 6415-6422.	13.7	51
96	Connecting the surface structure, morphology and photocatalytic activity of Ag2O: An in depth and unified theoretical investigation. Applied Surface Science, 2020, 509, 145321.	6.1	51
97	Spin-Philicity and Spin-Donicity as Auxiliary Concepts To Quantify Spin-Catalysis Phenomena. Journal of Physical Chemistry A, 2002, 106, 5353-5357.	2.5	50
98	Towards an insight on the photoluminescence of disordered CaWO4 from a joint experimental and theoretical analysis. Journal of Solid State Chemistry, 2005, 178, 1284-1291.	2.9	50
99	Photoluminescent properties of ZrO2: Tm3+, Tb3+, Eu3+ powdersâ€"A combined experimental and theoretical study. Journal of Alloys and Compounds, 2017, 695, 3094-3103.	5.5	50
100	SnO2 nanocrystals synthesized by microwave-assisted hydrothermal method: towards a relationship between structural and optical properties. Journal of Nanoparticle Research, 2012, 14, 1.	1.9	49
101	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.	3.3	49
102	Contribution of structural order-disorder to the green photoluminescence ofPbWO4. Physical Review B, 2007, 75, .	3.2	48
103	An Experimental and Computational Study of Î²-AgVO₃: Optical Properties and Formation of Ag Nanoparticles. Journal of Physical Chemistry C, 2016, 120, 12254-12264.	3.1	48
104	New insights on the bridge carbonâ€"carbon bond in propellanes: A theoretical study based on the analysis of the electron localization function. Journal of Computational Chemistry, 2007, 28, 857-864.	3.3	47
105	On the reversed crystal growth of BaZrO3 decaoctahedron: shape evolution and mechanism. CrystEngComm, 2011, 13, 5818.	2.6	47
106	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.	2.3	47
107	Nonlocal (Pair Site) Reactivity from Second-Order Static Density Response Function:â€‰ Gas- and Solution-Phase Reactivity of the Acetaldehyde Enolate as a Test Case. Journal of Physical Chemistry A, 1999, 103, 1367-1375.	2.5	46
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.	4.0	46

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109	A Comparative Study of Claisen and Cope Rearrangements Catalyzed by Chorismate Mutase. An Insight into Enzymatic Efficiency:Â Transition State Stabilization or Substrate Preorganization?. Journal of the American Chemical Society, 2004, 126, 311-319.	13.7	45
110	A theoretical study on the photoluminescence of SrTiO3. Chemical Physics Letters, 2010, 493, 141-146.	2.6	45
111	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.	3.1	45
112	Synthesis and morphological transformation of BaWO4 crystals: Experimental and theoretical insights. Ceramics International, 2016, 42, 10913-10921.	4.8	45
113	Magnetism and multiferroic properties at MnTiO3 surfaces: A DFT study. Applied Surface Science, 2018, 452, 463-472.	6.1	45
114	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.	3.1	45
115	A theoretical study of water adsorption on (10-10) and (0001) ZnO surfaces: molecular cluster, basis set and effective core potential dependence. Computational and Theoretical Chemistry, 1995, 330, 347-351.	1.5	44
116	Theoretical Study of the Elimination Kinetics of Carboxylic Acid Derivatives in the Gas Phase. Decomposition of 2-Chloropropionic Acid. Journal of Physical Chemistry A, 1997, 101, 1859-1865.	2.5	44
117	Transition structure selectivity in enzyme catalysis: a QM/MM study of chorismate mutase. Theoretical Chemistry Accounts, 2001, 105, 207-212.	1.4	44
118	DFT Study of Oxygen Adsorption on Modified Nanostructured Gold Pyramids. Journal of Physical Chemistry B, 2005, 109, 7624-7630.	2.6	44
119	Nature of the ringâ€closure process along the rearrangement of octaâ€1,3,5,7â€tetraene to cyclooctaâ€1,3,5â€triene from the perspective of the electron localization function and catastrophe theory. Journal of Computational Chemistry, 2012, 33, 748-756.	3.3	44
120	Improving the ozone gas-sensing properties of CuWO4 nanoparticles. Journal of Alloys and Compounds, 2018, 748, 411-417.	5.5	44
121	Unvealing the role of Î²-Ag2MoO4 microcrystals to the improvement of antibacterial activity. Materials Science and Engineering C, 2020, 111, 110765.	7.3	44
122	Enzyme catalysis and transition structures in vacuo. Transition structures for the enolization, carboxylation and oxygenation reactions in ribulose-1,5-bisphosphate carboxylase/oxygenase enzyme (Rubisco). Journal of the Chemical Society, Faraday Transactions, 1994, 90, 2365-2374.	1.7	43
123	Quantum-mechanical simulation ofMgAl2O4under high pressure. Physical Review B, 2002, 66, .	3.2	43
124	On the Nature of the Transition State in CatecholO-Methyltransferase. A Complementary Study Based on Molecular Dynamics and Potential Energy Surface Explorations. Journal of the American Chemical Society, 2005, 127, 10648-10655.	13.7	43
125	Toward an Understanding of the Catalytic Role of Hydrogen-Bond Donor Solvents in the Hetero-Dielsâ€Alder Reaction between Acetone and Butadiene Derivative. Journal of Physical Chemistry A, 2005, 109, 10438-10444.	2.5	43
126	Migration of the subsurfaceCimpurity inPd(111). Physical Review B, 2005, 71, .	3.2	43

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127	Oxygen adsorption on gold nanofacets and model clusters. Journal of Chemical Physics, 2006, 125, 054703.	3.0	43
128	A <scp>DFT</scp> Study of Structural and Electronic Properties of <scp><scp>ZnS</scp></scp> Polymorphs and its Pressureâ€Induced Phase Transitions. Journal of the American Ceramic Society, 2014, 97, 4011-4018.	3.8	43
129	Electronic aspects of LADH catalytic mechanism. International Journal of Quantum Chemistry, 1991, 39, 767-786.	2.0	42
130	Theoretical Study of Transition Structures for Intramolecular Hydrogen Transfer in Molecular Models Representing D-Ribulose 1,5-Bisphosphate. A Possible Molecular Mechanism for the Enolization Step in Rubisco. The Journal of Physical Chemistry, 1994, 98, 4821-4830.	2.9	42
131	H2O and H2 interaction with ZnO surfaces: A MNDO, AM1, and PM3 theoretical study with large cluster models. International Journal of Quantum Chemistry, 1996, 57, 861-870.	2.0	42
132	A theoretical analysis of the TiO2/Sn doped (110) surface properties. Surface Science, 2005, 580, 71-79.	1.9	42
133	Towards the scale-up of the formation of nanoparticles on Î±-Ag2WO4 with bactericidal properties by femtosecond laser irradiation. Scientific Reports, 2018, 8, 1884.	3.3	42
134	Experimental and theoretical study to explain the morphology of CaMoO 4 crystals. Journal of Physics and Chemistry of Solids, 2018, 114, 141-152.	4.0	42
135	Theoretical approach for determining the relation between the morphology and surface magnetism of Co3O4. Journal of Magnetism and Magnetic Materials, 2018, 453, 262-267.	2.3	42
136	A Theoretical Study of the Reaction between Cyclopentadiene and Protonated Imine Derivatives:Â A Shift from a Concerted to a Stepwise Molecular Mechanism. Journal of Organic Chemistry, 2001, 66, 6151-6157.	3.2	41
137	Topological analysis of the bonds in incomplete cuboidal [Mo3S4] clusters. New Journal of Chemistry, 2002, 26, 844-850.	2.8	41
138	An electron localization function and catastrophe theory analysis on the molecular mechanism of gas-phase identity SN2 reactions. Theoretical Chemistry Accounts, 2008, 120, 341-349.	1.4	41
139	Computational design of biological catalysts. Chemical Society Reviews, 2008, 37, 2634.	38.1	41
140	Flexural behavior and water absorption of asymmetrical sandwich composites from natural fibers and cork agglomerate core. Materials Letters, 2014, 127, 48-52.	2.6	41
141	In situ Transmission Electron Microscopy observation of Ag nanocrystal evolution by surfactant free electron-driven synthesis. Scientific Reports, 2016, 6, 21498.	3.3	41
142	SiO2-Ag Composite as a Highly Virucidal Material: A Roadmap that Rapidly Eliminates SARS-CoV-2. Nanomaterials, 2021, 11, 638.	4.1	41
143	Ag Nanoparticles/Î±-Ag2WO4 Composite Formed by Electron Beam and Femtosecond Irradiation as Potent Antifungal and Antitumor Agents. Scientific Reports, 2019, 9, 9927.	3.3	40
144	Theoretical study of solvation effects on chemical reactions. A combined quantum chemical/Monte Carlo study of the Meyer-Schuster reaction mechanism in water. Journal of the American Chemical Society, 1989, 111, 829-835.	13.7	39

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145	Prediction of Gold Zigzag Nanotube-like Structure Based on Au32Units: A Quantum Chemical Study. Journal of Physical Chemistry C, 2007, 111, 10342-10346.	3.1	39
146	A Quantum Mechanics/Molecular Mechanics Study of the Proteinâ€“Ligand Interaction for Inhibitors of HIV-1 Integrase. Chemistry - A European Journal, 2007, 13, 7715-7724.	3.3	38
147	CaSO₄ and Its Pressure-Induced Phase Transitions. A Density Functional Theory Study. Inorganic Chemistry, 2012, 51, 1751-1759.	4.0	38
148	Formation of Ag Nanoparticles on Î²-Ag₂WO₄ through Electron Beam Irradiation: A Synergetic Computational and Experimental Study. Inorganic Chemistry, 2016, 55, 8661-8671.	4.0	38
149	Combined Experimental and Theoretical Study to Understand the Photoluminescence of Sr1-xTiO3-x. Journal of Physical Chemistry B, 2004, 108, 9221-9227.	2.6	37
150	Strain behavior of lanthanum modified BiFeO3 thin films prepared via soft chemical method. Journal of Applied Physics, 2008, 104, 104115.	2.5	37
151	Microwave-hydrothermal synthesis of single-crystalline Co3O4 spinel nanocubes. CrystEngComm, 2013, 15, 7443.	2.6	37
152	Theoretical study of the structure and stability of NbxOy and NbxOy+ (x=1â€“3; y=2â€“5,â€ˆ7,â€ˆ8) clusters. Chemical Physics Letters, 1998, 287, 620-626.	2.6	36
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