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	Crystal growth in colloidal tin oxide nanocrystals induced by coalescence at room temperature. Applied Physics Letters, 2003, 83, 1566-1568.	1.5	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.	3.8	194
3	Morphology and Blue Photoluminescence Emission of PbMoO₄ Processed in Conventional Hydrothermal. Journal of Physical Chemistry C, 2009, 113, 5812-5822.	1.5	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.	1.1	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.	2.3	152
6	Theoretical insights in enzyme catalysis. Chemical Society Reviews, 2004, 33, 98-107.	18.7	150
7	Electronic structure and optical properties of BaMoO4 powders. Current Applied Physics, 2010, 10, 614-624.	1.1	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.	1.1	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.	1.7	136
10	Hierarchical Assembly of CaMoO₄ Nano-Octahedrons and Their Photoluminescence Properties. Journal of Physical Chemistry C, 2011, 115, 5207-5219.	1.5	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.	1.1	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.	1.5	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.	2.1	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.	1.5	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.	1.2	119
16	Static simulation of bulk and selected surfaces of anatase TiO2. Surface Science, 2001, 490, 116-124.	0.8	115
17	Thermodynamic argument about SnO2 nanoribbon growth. Applied Physics Letters, 2003, 83, 635-637.	1.5	115
18	Nine questions on energy decomposition analysis. Journal of Computational Chemistry, 2019, 40, 2248-2283.	1.5	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.	1.3	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.	1.1	107
21	Synthesis of wurtzite ZnS nanoparticles using the microwave assisted solvothermal method. Journal of Alloys and Compounds, 2013, 556, 153-159.	2.8	105
22	A novel ozone gas sensor based on one-dimensional (1D) Î±-Ag₂WO₄ nanostructures. Nanoscale, 2014, 6, 4058-4062.	2.8	105
23	Room-temperature photoluminescence ofBaTiO3:â€ƒJoint experimental and theoretical study. Physical Review B, 2005, 71, .	1.1	103
24	Direct in situ observation of the electron-driven synthesis of Ag filaments on Î±-Ag2WO4 crystals. Scientific Reports, 2013, 3, 1676.	1.6	103
25	ZnWO₄ nanocrystals: synthesis, morphology, photoluminescence and photocatalytic properties. Physical Chemistry Chemical Physics, 2018, 20, 1923-1937.	1.3	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.	0.8	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.	1.1	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.	1.3	100
29	Potentiated Electron Transference in Î±-Ag₂WO₄ Microcrystals with Ag Nanofilaments as Microbial Agent. Journal of Physical Chemistry A, 2014, 118, 5769-5778.	1.1	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.	1.6	99
31	Density functional theory calculation of the electronic structure ofBa0.5Sr0.5TiO3:Photoluminescent properties and structural disorder. Physical Review B, 2004, 69, .	1.1	98
32	A relationship between structural and electronic orderâ€“disorder effects and optical properties in crystalline TiO₂nanomaterials. Dalton Transactions, 2015, 44, 3159-3175.	1.6	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.	1.7	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.	6.6	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.	1.7	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.	1.3	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.	1.4	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, .	1.1	84
39	Unraveling reaction mechanisms by means of Quantum Chemical Topology Analysis. International Journal of Quantum Chemistry, 2014, 114, 1239-1252.	1.0	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.	1.3	84
41	A combined theoretical and experimental study of electronic structure and optical properties of Î²-ZnMoO4 microcrystals. Polyhedron, 2013, 54, 13-25.	1.0	83
42	Silver Molybdate and Silver Tungstate Nanocomposites with Enhanced Photoluminescence. Nanomaterials and Nanotechnology, 2014, 4, 22.	1.2	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.	1.2	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.	6.6	79
45	Describing the Molecular Mechanism of Organic Reactions by Using Topological Analysis of Electronic Localization Function. Current Organic Chemistry, 2011, 15, 3566-3575.	0.9	79
46	The interplay between morphology and photocatalytic activity in ZnO and N-doped ZnO crystals. Materials and Design, 2017, 120, 363-375.	3.3	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.	6.6	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.	1.5	76
49	Protective Face Masks: Current Status and Future Trends. ACS Applied Materials & Interfaces, 2021, 13, 56725-56751.	4.0	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.	1.1	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.	1.2	73
52	A Joint Experimental and Theoretical Study on the Nanomorphology of CaWO₄ Crystals. Journal of Physical Chemistry C, 2011, 115, 20113-20119.	1.5	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.	1.2	72
54	An efficient microwave-assisted hydrothermal synthesis of BaZrO3 microcrystals: growth mechanism and photoluminescence emissions. CrystEngComm, 2010, 12, 3612.	1.3	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.	1.1	71
56	Electronic and structural properties of SnxTi1â^'xO2 solid solutions: a periodic DFT study. Catalysis Today, 2003, 85, 145-152.	2.2	71
57	A theoretical analysis of adsorption and dissociation of CH3OH on the stoichiometric SnO2(110) surface. Surface Science, 1999, 430, 213-222.	0.8	70
58	Photoluminescence and Photocatalytic Properties of Ag₃PO₄ Microcrystals: An Experimental and Theoretical Investigation. ChemPlusChem, 2016, 81, 202-212.	1.3	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.	0.5	69
60	An improved method for preparation of SrTiO3 nanoparticles. Materials Chemistry and Physics, 2011, 125, 168-173.	2.0	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.	6.6	68
62	Quantum-mechanical analysis of the equation of state of anataseTiO2. Physical Review B, 2001, 64, .	1.1	68
63	Theoretical Study on the Molecular Mechanism for the Reaction of VO2+ with C2H4. Journal of Physical Chemistry A, 2003, 107, 3107-3120.	1.1	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.	1.3	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.	6.6	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.	2.2	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.	2.8	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.	1.1	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.	0.5	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.	1.1	64
71	Structural refinement, growth mechanism, infrared/Raman spectroscopies and photoluminescence properties of PbMoO4 crystals. Polyhedron, 2013, 50, 532-545.	1.0	63
72	Quantum Mechanics Insight into the Microwave Nucleation of SrTiO₃ Nanospheres. Journal of Physical Chemistry C, 2012, 116, 24792-24808.	1.5	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.	1.1	62
74	A theoretical study on cytosine tautomers in aqueous media by using continuum models. Chemical Physics Letters, 2000, 317, 437-443.	1.2	61
75	DFT Study of the Reaction between VO2+ and C2H6. Organometallics, 2004, 23, 730-739.	1.1	61
76	Unveiling the Chemical and Morphological Features of Sbâˆ’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.	6.6	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.	1.1	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.	2.8	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.	6.6	60
80	Origin of photoluminescence in SrTiO3: a combined experimental and theoretical study. Journal of Solid State Chemistry, 2004, 177, 3879-3885.	1.4	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.	1.3	60
82	Surfactant-Mediated Morphology and Photocatalytic Activity of Î±-Ag₂WO₄ Material. Journal of Physical Chemistry C, 2018, 122, 8667-8679.	1.5	60
83	Nucleophilicity Index from Perturbed Electrostatic Potentials. Journal of Physical Chemistry A, 2007, 111, 2442-2447.	1.1	59
84	Preorganization and Reorganization as Related Factors in Enzyme Catalysis: The Chorismate Mutase Case. Chemistry - A European Journal, 2003, 9, 984-991.	1.7	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.	1.1	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.	1.5	56
87	First-Principles Study of Pressure-Induced Phase Transitions and Electronic Properties of Ag₂MoO₄. Journal of Physical Chemistry C, 2014, 118, 3724-3732.	1.5	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.	1.2	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.	1.2	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.	1.3	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.	0.8	53
92	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
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.	10.8	53
94	Lithium insertion and mobility in the TiO2-anatase/titanate structure: A periodic DFT study. Journal of Electroanalytical Chemistry, 2005, 581, 216-223.	1.9	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.	6.6	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.	3.1	51
97	Spin-Philicity and Spin-Donicity as Auxiliary Concepts To Quantify Spin-Catalysis Phenomena. Journal of Physical Chemistry A, 2002, 106, 5353-5357.	1.1	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.	1.4	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.	2.8	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.	0.8	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.	1.6	49
102	Contribution of structural order-disorder to the green photoluminescence ofPbWO4. Physical Review B, 2007, 75, .	1.1	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.	1.5	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.	1.5	47
105	On the reversed crystal growth of BaZrO3 decaoctahedron: shape evolution and mechanism. CrystEngComm, 2011, 13, 5818.	1.3	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.	1.2	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.	1.1	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.	1.9	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.	6.6	45
110	A theoretical study on the photoluminescence of SrTiO3. Chemical Physics Letters, 2010, 493, 141-146.	1.2	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.	1.5	45
112	Synthesis and morphological transformation of BaWO4 crystals: Experimental and theoretical insights. Ceramics International, 2016, 42, 10913-10921.	2.3	45
113	Magnetism and multiferroic properties at MnTiO3 surfaces: A DFT study. Applied Surface Science, 2018, 452, 463-472.	3.1	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.	1.5	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.	1.1	44
117	Transition structure selectivity in enzyme catalysis: a QM/MM study of chorismate mutase. Theoretical Chemistry Accounts, 2001, 105, 207-212.	0.5	44
118	DFT Study of Oxygen Adsorption on Modified Nanostructured Gold Pyramids. Journal of Physical Chemistry B, 2005, 109, 7624-7630.	1.2	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.	1.5	44
120	Improving the ozone gas-sensing properties of CuWO4 nanoparticles. Journal of Alloys and Compounds, 2018, 748, 411-417.	2.8	44
121	Unvealing the role of Î²-Ag2MoO4 microcrystals to the improvement of antibacterial activity. Materials Science and Engineering C, 2020, 111, 110765.	3.8	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, .	1.1	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.	6.6	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.	1.1	43
126	Migration of the subsurfaceCimpurity inPd(111). Physical Review B, 2005, 71, .	1.1	43

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127	Oxygen adsorption on gold nanofacets and model clusters. Journal of Chemical Physics, 2006, 125, 054703.	1.2	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.	1.9	43
129	Electronic aspects of LADH catalytic mechanism. International Journal of Quantum Chemistry, 1991, 39, 767-786.	1.0	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.	1.0	42
132	A theoretical analysis of the TiO2/Sn doped (110) surface properties. Surface Science, 2005, 580, 71-79.	0.8	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.	1.6	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.	1.9	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.	1.0	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.	1.7	41
137	Topological analysis of the bonds in incomplete cuboidal [Mo3S4] clusters. New Journal of Chemistry, 2002, 26, 844-850.	1.4	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.	0.5	41
139	Computational design of biological catalysts. Chemical Society Reviews, 2008, 37, 2634.	18.7	41
140	Flexural behavior and water absorption of asymmetrical sandwich composites from natural fibers and cork agglomerate core. Materials Letters, 2014, 127, 48-52.	1.3	41
141	In situ Transmission Electron Microscopy observation of Ag nanocrystal evolution by surfactant free electron-driven synthesis. Scientific Reports, 2016, 6, 21498.	1.6	41
142	SiO2-Ag Composite as a Highly Virucidal Material: A Roadmap that Rapidly Eliminates SARS-CoV-2. Nanomaterials, 2021, 11, 638.	1.9	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.	1.6	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.	6.6	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.	1.5	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.	1.7	38
147	CaSO₄ and Its Pressure-Induced Phase Transitions. A Density Functional Theory Study. Inorganic Chemistry, 2012, 51, 1751-1759.	1.9	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.	1.9	38
149	Combined Experimental and Theoretical Study to Understand the Photoluminescence of Sr1-xTiO3-x. Journal of Physical Chemistry B, 2004, 108, 9221-9227.	1.2	37
150	Strain behavior of lanthanum modified BiFeO3 thin films prepared via soft chemical method. Journal of Applied Physics, 2008, 104, 104115.	1.1	37
151	Microwave-hydrothermal synthesis of single-crystalline Co3O4 spinel nanocubes. CrystEngComm, 2013, 15, 7443.	1.3	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.	1.2	36
153	The nature of the chemical bond in di- and polynuclear metal cluster complexes as depicted by the analysis of the electron localization function. Comptes Rendus Chimie, 2005, 8, 1400-1412.	0.2	36
154	Molecular oxygen adsorption on electropositive nano gold tips. Chemical Physics Letters, 2006, 421, 433-438.	1.2	36
155	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
156	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
157	Structural properties and self-activated photoluminescence emissions in hydroxyapatite with distinct particle shapes. Ceramics International, 2018, 44, 236-245.	2.3	36
158	Theoretical study of ZnO (1010) and Cu/ZnO (1010) surfaces. Chemical Physics Letters, 2001, 338, 224-230.	1.2	35
159	A DFT study of the Dielsâ€“Alder reaction between methyl acrolein derivatives and cyclopentadiene. Understanding the effects of Lewis acids catalysts based on sulfur containing boron heterocycles. Tetrahedron, 2006, 62, 5502-5509.	1.0	35
160	A Theoretical Study on the Pressure-Induced Phase Transitions in the Inverse Spinel Structure Zn₂SnO₄. Journal of Physical Chemistry C, 2011, 115, 7740-7746.	1.5	35
161	Anomalous oriented attachment growth behavior on SnO2 nanocrystals. Chemical Communications, 2011, 47, 3117.	2.2	35
162	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

#	Article	IF	Citations
163	Radioluminescence properties of decaoctahedral BaZrO3. Scripta Materialia, 2011, 64, 118-121.	2.6	34
164	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
165	Structure, morphology and photoluminescence emissions of ZnMoO4: RE 3+=Tb3+ - Tm3+ - X Eu3+ (xÂ= 1,) Tj ETQq1 1 0.784314 rgBT Compounds, 2018, 750, 55-70.	2.8	34
166	Theoretical study of the solvent effects on the mechanisms of addition of dimethyl acetylenedicarboxylate to 1-methyl-2-vinylpyrrole. Tetrahedron, 1996, 52, 10693-10704.	1.0	33
167	Comparative theoretical study of transition structures, barrier heights, and reaction energies for the intramolecular tautomerization in acetaldehyde/vinyl alcohol and acetaldimine/vinylamine systems. International Journal of Quantum Chemistry, 1998, 66, 9-24.	1.0	33
168	Theoretical Study of the Mechanisms for the Alkoxyacetic Acids Decomposition. Journal of Physical Chemistry A, 1999, 103, 3935-3943.	1.1	33
169	Density functional study of the 5-methylcytosine tautomers. Chemical Physics, 2001, 264, 333-340.	0.9	33
170	Effect of electron-withdrawing substituents on the electrophilicity of carbonyl carbons. Tetrahedron, 2005, 61, 417-422.	1.0	33
171	Theoretical kinetic isotope effects for the hydride-transfer step in lactate dehydrogenase. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 1703-1707.	1.7	32
172	On Transition Structures for Hydride Transfer Step: A Theoretical Study of the Reaction Catalyzed by Dihydrofolate Reductase Enzyme. Bioorganic Chemistry, 1996, 24, 10-18.	2.0	32
173	Ab InitioStudy of Stereo- and Regioselectivity in the Dielsâ^'Alder Reaction between 2-Phenylcyclopentadiene and Î±-(Methylthio)acrylonitrile. Journal of Organic Chemistry, 1997, 62, 1775-1778.	1.7	32
174	Potential energy surface for the decomposition of mandelic acid. Chemical Physics Letters, 1997, 274, 422-428.	1.2	32
175	Relationship between nucleophilicity/electrophilicity indices and reaction mechanisms for the nucleophilic substitution reactions of carbonyl compounds. Journal of Physical Organic Chemistry, 2004, 17, 273-281.	0.9	32
176	How a Quantum Chemical Topology Analysis Enables Prediction of Electron Density Transfers in Chemical Reactions. The Degenerated Cope Rearrangement of Semibullvalene. Journal of Physical Chemistry Letters, 2012, 3, 2500-2505.	2.1	32
177	Lewis Acid and Substituent Effects on the Molecular Mechanism for the Nazarov Reaction of Penta-1,4-dien-3-one and Derivatives. A Topological Analysis Based on the Combined Use of Electron Localization Function and Catastrophe Theory. Journal of Chemical Theory and Computation, 2007, 3, 816-823.	2.3	31
178	Origin of the Absorption Maxima of the Photoactive Yellow Protein Resolved via Ab Initio Multiconfigurational Methods. Journal of Physical Chemistry B, 2008, 112, 7153-7156.	1.2	31
179	Correlation between structural and electronic orderâ€“disorder effects and optical properties in ZnO nanocrystals. Journal of Materials Chemistry C, 2014, 2, 10164-10174.	2.7	31
180	Theoretical and Experimental Insight on Ag₂CrO₄ Microcrystals: Synthesis, Characterization, and Photoluminescence Properties. Inorganic Chemistry, 2016, 55, 8961-8970.	1.9	31

#	Article	IF	Citations
181	Formation of Ag nanoparticles on metastable Î²-Ag2WO4 microcrystals induced by electron irradiation. Chemical Physics Letters, 2016, 644, 68-72.	1.2	31
182	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
183	The nature of the Auâ€“Rg bond in the [AuRg 4] 2+ (Rg=Ar, Kr and Xe) molecules. Chemical Physics Letters, 2002, 356, 483-489.	1.2	30
184	Photoluminescent behavior of SrZrO3/SrTiO3 multilayer thin films. Chemical Physics Letters, 2009, 473, 293-298.	1.2	30
185	Toward Understanding the Photochemistry of Photoactive Yellow Protein: A CASPT2/CASSCF and Quantum Theory of Atoms in Molecules Combined Study of a Model Chromophore in Vacuo. Journal of Chemical Theory and Computation, 2009, 5, 3032-3038.	2.3	30
186	Manufacture of Green-Composite Sandwich Structures with Basalt Fiber and Bioepoxy Resin. Advances in Materials Science and Engineering, 2013, 2013, 1-9.	1.0	30
187	In situgrowth of Ag nanoparticles onÎ±-Ag₂WO₄under electron irradiation: probing the physical principles. Nanotechnology, 2016, 27, 225703.	1.3	30
188	Synthesis and evaluation of Î±-Ag2WO4 as novel antifungal agent. Chemical Physics Letters, 2017, 674, 125-129.	1.2	30
189	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
190	A theoretical study of the singlet-triplet energy gap dependence upon rotation and pyramidalization for 1,2-dihydroxyethylene: a simple model to study the enediol moiety in Rubisco's substrate. The Journal of Physical Chemistry, 1993, 97, 7888-7893.	2.9	29
191	Transition state structure invariance to model system size and calculation levels: a QM/MM study of the carboxylation step catalyzed by Rubisco. Theoretical Chemistry Accounts, 1999, 101, 228-233.	0.5	29
192	Effect of Coverage and Defects on the Adsorption of Propanethiol on Au(111) Surface: A Theoretical Study. Langmuir, 2011, 27, 14514-14521.	1.6	29
193	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
194	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
195	A theoretical study of (1010) and (0001) ZnO surfaces: molecular cluster model, basis set and effective core potential dependence. Computational and Theoretical Chemistry, 1995, 330, 301-306.	1.5	28
196	Molecular Structure of the Molybdenum Oxo-Diperoxo Compound MoO(O2)2(OPy)(H2O):Â A Computational and X-ray Study. Inorganic Chemistry, 2001, 40, 6022-6025.	1.9	28
197	Mechanistic Insights into the Reaction between VO2+ and Propene Based on a DFT Study. Organometallics, 2006, 25, 1643-1653.	1.1	28
198	Catalysis in Glycine N-Methyltransferase:â€‰ Testing the Electrostatic Stabilization and Compression Hypothesis. Biochemistry, 2006, 45, 14917-14925.	1.2	28

#	Article	IF	Citations
199	Mechanism and Plasticity of Isochorismate Pyruvate Lyase: A Computational Study. Journal of the American Chemical Society, 2009, 131, 16156-16161.	6.6	28
200	Relationship between Crystal Shape, Photoluminescence, and Local Structure in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SrTiO</mml:mtext></mml:mrow> by Microwave-Assisted Hydrothermal Method. Journal of Nanomaterials, 2012, 2012, 1-6.	1.5	28
201	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.	1.5	28
202	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
203	An ab initio perturbed ion study of structural properties of TiO2, SnO2 and GeO2 rutile lattices. Chemical Physics, 1996, 212, 381-391.	0.9	27
204	Understanding the Nature of the Molecular Mechanisms Associated with the Competitive Lewis Acid Catalyzed[4+2] and[4+3] Cycloadditions between Arylidenoxazolone Systems and Cyclopentadiene: A DFT Analysis. Chemistry - A European Journal, 2004, 10, 4742-4749.	1.7	27
205	A Theoretical Study on the Electronic Structure of Auâ^'XO(0,-1,+1)Â(X = C, N, and O) Complexes:Â Effect of an External Electric Field. Journal of Physical Chemistry A, 2007, 111, 13255-13263.	1.1	27
206	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
207	Straining the double bond in 1,2-dihydroxyethylene. A simple theoretical model for the enediol moiety in Rubisco's substrate and analogs. Chemical Physics Letters, 1992, 198, 515-520.	1.2	26
208	Transition structure for the hydride transfer reaction from formate anion to cyclopropenyl cation: a simple theoretical model for the reaction catalyzed by formate dehydrogenase. Chemical Physics Letters, 1992, 189, 395-400.	1.2	26
209	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.	1.1	26
210	Electronic fluxes during dielsâ€alder reactions involving 1,2â€benzoquinones: mechanistic insights from the analysis of electron localization function and catastrophe theory. Journal of Computational Chemistry, 2012, 33, 2400-2411.	1.5	26
211	Electronic structure and magnetic properties of FeWO4 nanocrystals synthesized by the microwave-hydrothermal method. Materials Characterization, 2012, 73, 124-129.	1.9	26
212	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
213	Electronic aspects of the hydride transfer mechanism.Abinitioanalytical gradient studies of the cyclopropenylâ€cation/lithium hydride model reactant system. Journal of Chemical Physics, 1985, 83, 4673-4682.	1.2	25
214	A Theoretical Study of Addition of Organomagnesium Reagents to Chiral Î±-Alkoxy Carbonyl Compounds. Journal of Organic Chemistry, 1996, 61, 3467-3475.	1.7	25
215	A combined experimental and theoretical study of the unimolecular elimination kinetics of 2-alkoxypropionic acids in the gas phase. Chemical Physics, 1999, 246, 1-12.	0.9	25
216	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.	1.2	25

#	Article	IF	Citations
217	Nucleofugality index in Î±-elimination reactions. Chemical Physics Letters, 2007, 439, 177-182.	1.2	25
218	Intercalation processes and diffusion paths of lithium ions in spinel-type structured<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Li</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>+</mml:mo><mml:mi>x</mml:mi></mml:mrow></m mathvariant="normal">Ti</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math>: Density functional theory. Physical Review B, 2008, 77, .	1.1	25
219	Predicting an Improvement of Secondary Catalytic Activity of Promiscuos Isochorismate Pyruvate Lyase by Computational Design. Journal of the American Chemical Society, 2008, 130, 2894-2895.	6.6	25
220	Insight into Copperâ€Based Catalysts: Microwaveâ€Assisted Morphosynthesis, Inâ€…Situ Reduction Studies, and Dehydrogenation of Ethanol. ChemCatChem, 2011, 3, 839-843.	1.8	25
221	Am1 and pm3 transition structure for the hydride transfer. A model of reaction catalyzed by dihydrofolate reductase. Computational and Theoretical Chemistry, 1995, 330, 411-416.	1.5	24
222	A theoretical study of the molecular mechanism for the oxidation of methanol by PQQ. Journal of the American Chemical Society, 1995, 117, 8807-8815.	6.6	24
223	On Transition Structures for Hydride Transfer Step in Enzyme Catalysis. A Comparative Study on Models of Glutathione Reductase Derived from Semiempirical, HF, and DFT Methods. Journal of Organic Chemistry, 1996, 61, 7777-7783.	1.7	24
224	A Theoretical Study of the Favorskii Rearrangement. Calculation of Gas-Phase Reaction Paths and Solvation Effects on the Molecular Mechanism for the Transposition of the Î±-Chlorocyclobutanone. Journal of the American Chemical Society, 1997, 119, 1941-1947.	6.6	24
225	A B3LYP/6-31G** study on the chlorination of ammonia by hypochlorous acid. Chemical Physics Letters, 2001, 342, 405-410.	1.2	24
226	Sulfide and Sulfoxide Oxidations by Mono- and Diperoxo Complexes of Molybdenum. A Density Functional Study. Journal of Organic Chemistry, 2003, 68, 5870-5874.	1.7	24
227	Toward Understanding the Electron Density Distribution in Magnetic Clusters:Â Insight from the ELF and AIM Analyses of Ground-State Fe4. Journal of Physical Chemistry A, 2004, 108, 6025-6031.	1.1	24
228	Better Understanding of the Ring-Cleavage Process of Cyanocyclopropyl Anionic Derivatives. A Theoretical Study Based on the Electron Localization Function. Journal of Organic Chemistry, 2006, 71, 754-762.	1.7	24
229	Computer-Aided Rational Design of Catalytic Antibodies: The 1F7 Case. Angewandte Chemie - International Edition, 2007, 46, 286-290.	7.2	24
230	Effects of chemical substitution on the structural and optical properties of Î±-Ag_{2â^'2x}Ni_xWO₄ (0 â‰¤ x â‰¤ 0.08) solid solutions. Physical Chemistry Chemical Physics, 2016, 18, 21966-21975.	1.3	24
231	On the morphology of BaMoO₄ crystals: A theoretical and experimental approach. Crystal Research and Technology, 2016, 51, 634-644.	0.6	24
232	Synthesis and characterization of metastable Î²-Ag₂WO₄: an experimental and theoretical approach. Dalton Transactions, 2016, 45, 1185-1191.	1.6	24
233	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
234	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

#	Article	IF	Citations
235	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
236	Towards an explanation of carboxylation/oxygenation bifunctionality in Rubisco. Transition structure for the carboxylation reaction of 2,3,4-pentanetriol. Molecular Engineering, 1992, 2, 37-41.	0.2	23
237	Ab initio cluster-in-the-lattice description of vanadium-doped zircon: analysis of the impurity centers in vanadium(4+)-doped zircon (ZrSiO4). The Journal of Physical Chemistry, 1993, 97, 2555-2559.	2.9	23
238	Ab initio study of CO and H2 interaction on ZnO surfaces using a small cluster model. Computational and Theoretical Chemistry, 1997, 398-399, 457-466.	1.5	23
239	A Quantum Mechanic/Molecular Mechanic Study of the Wild-Type and N155S Mutant HIV-1 Integrase Complexed with Diketo Acid. Biophysical Journal, 2008, 94, 2443-2451.	0.2	23
240	Olefin Epoxidation by Molybdenum Peroxo Compound: Molecular Mechanism Characterized by the Electron Localization Function and Catastrophe Theory. Journal of Physical Chemistry A, 2011, 115, 514-522.	1.1	23
241	Combined Theoretical and Experimental Analysis of the Bonding in the Heterobimetallic Cubane-Type Mo3NiS4and Mo3CuS4Core Clusters. Inorganic Chemistry, 2007, 46, 2159-2166.	1.9	22
242	Synthesis, optical and ferroelectric properties of PZT thin films: experimental and theoretical investigation. Journal of Materials Chemistry, 2012, 22, 6587.	6.7	22
243	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
244	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
245	Uncovering the metastable Î³-Ag₂WO₄phase: a joint experimental and theoretical study. RSC Advances, 2017, 7, 5610-5620.	1.7	22
246	Experimental and theoretical study of the energetic, morphological, and photoluminescence properties of CaZrO₃:Eu³⁺. CrystEngComm, 2018, 20, 5519-5530.	1.3	22
247	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
248	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
249	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
250	Transition structures in vacuo and the theory of enzyme catalysis. Rubisco's catalytic mechanism: a paradigmatic case?. Computational and Theoretical Chemistry, 1995, 342, 131-140.	1.5	21
251	Theoretical analysis of the energy levels induced by oxygen vacancies and the doping process (Co, Cu) Tj ETQq1 1 0.784314 rgBT /Ov	1.5	21
252	An atom-in-molecules and electron-localization-function study of the interaction between O 2 and V x O y + /V x O y (x = 1, 2, y = 1-5) clusters. Theoretical Chemistry Accounts, 2002, 108, 12-20.	0.5	21

#	Article	IF	Citations
253	Novel SrTi1â^'xFexO3 nanocubes synthesized by microwave-assisted hydrothermal method. CrystEngComm, 2012, 14, 4068.	1.3	21
254	Effect of polyvinyl alcohol on the shape, photoluminescence and photocatalytic properties of PbMoO4 microcrystals. Materials Science in Semiconductor Processing, 2014, 26, 425-430.	1.9	21
255	Î±- and Î²-AgVO3 polymorphs as photoluminescent materials: An example of temperature-driven synthesis. Ceramics International, 2018, 44, 5939-5944.	2.3	21
256	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
257	Carbon Nanofibers versus Silver Nanoparticles: Time-Dependent Cytotoxicity, Proliferation, and Gene Expression. Biomedicines, 2021, 9, 1155.	1.4	21
258	True and Apparent Oxygen Permeabilities of Contact Lenses. Optometry and Vision Science, 1992, 69, 685-690.	0.6	20
259	Why Do Peroxomolybdenum Complexes Chemoselectively Oxidize the Sulfur Centers of Unsaturated Sulfides and Sulfoxides? A DFT Analysis. European Journal of Organic Chemistry, 2005, 2005, 2406-2415.	1.2	20
260	Laser and electron beam-induced formation of Ag/Cr structures on Ag₂CrO₄. Physical Chemistry Chemical Physics, 2019, 21, 6101-6111.	1.3	20
261	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
262	Reading at exposed surfaces: theoretical insights into photocatalytic activity of ZnWO4. , 0, 1, 1005.		20
263	Electronic aspects of the hydride transfer mechanism. Computational and Theoretical Chemistry, 1988, 167, 395-412.	1.5	19
264	Quantum chemical study of the adsorption of water on zinc oxide surface. Computational and Theoretical Chemistry, 1994, 303, 19-24.	1.5	19
265	On a quantum theory of chemical reactions and the role of in vacuum transition structures. Primary and secondary sources of enzyme catalysis. Computational and Theoretical Chemistry, 1995, 335, 267-286.	1.5	19
266	Quantum Mechanical/Molecular Mechanical Study on the Favorskii Rearrangement in Aqueous Media. Journal of Physical Chemistry B, 2001, 105, 2453-2460.	1.2	19
267	Theoretical and experimental study of the relation between photoluminescence and structural disorder in barium and strontium titanate thin films. Journal of the European Ceramic Society, 2005, 25, 2337-2340.	2.8	19
268	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.	1.5	19
269	Hybrid Schemes Based on Quantum Mechanics/Molecular Mechanics Simulations. Advances in Protein Chemistry and Structural Biology, 2011, 85, 81-142.	1.0	19
270	Dopant Segregation Analysis on Sb:SnO₂ Nanocrystals. Chemistry - A European Journal, 2011, 17, 11515-11519.	1.7	19

#	ARTICLE	IF	CITATIONS
271	Structural and Electronic Properties of Lithiated SnO₂. A Periodic DFT Study. Journal of Physical Chemistry C, 2012, 116, 16127-16137.	1.5	19
272	From Complex Inorganic Oxides to Agâ€“Bi Nanoalloy: Synthesis by Femtosecond Laser Irradiation. ACS Omega, 2018, 3, 9880-9887.	1.6	19
273	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
274	Surface-dependent properties of Î±-Ag2WO4: a joint experimental and theoretical investigation. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	19
275	Modulating the properties of multifunctional semiconductors by means of morphology: Theory meets experiments. Computational Materials Science, 2021, 188, 110217.	1.4	19
276	HCnN: The largest molecules in the interstellar medium. Journal of Chemical Education, 1990, 67, 905.	1.1	18
277	A Theoretical Study of Stationary Structures for the Addition of Azide Anion to Tetrofuranosides: Modeling the Kinetic and Thermodynamic Controls by Solvent Effects. The Journal of Physical Chemistry, 1994, 98, 6955-6960.	2.9	18
278	Toward an Understanding of the Selectivity in Domino Reactions. A DFT Study of the Reaction between Acetylenedicarboxylic Acid and 1,3-Bis(2-furyl)propane. Journal of Organic Chemistry, 2000, 65, 3473-3477.	1.7	18
279	Photolumiscent Properties of Nanorods and Nanoplates Y2O3:Eu3+. Journal of Fluorescence, 2011, 21, 1431-1438.	1.3	18
280	Computational Chemistry Meets Experiments for Explaining the Geometry, Electronic Structure, and Optical Properties of Ca₁₀V₆O₂₅. Inorganic Chemistry, 2018, 57, 15489-15499.	1.9	18
281	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
282	Surface-dependent photocatalytic and biological activities of Ag2CrO4: Integration of experiment and simulation. Applied Surface Science, 2021, 545, 148964.	3.1	18
283	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
284	Amidine decomposition mechanism. A theoretical study. Computational and Theoretical Chemistry, 1992, 254, 465-472.	1.5	17
285	Rotational constants and dipole moments of interstellar polyynes: a comparative MP2 and density functional (BP86) study. Chemical Physics, 1996, 206, 57-61.	0.9	17
286	Transition structures of carbon dioxide fixation, hydration and C2 inversion for a model of Rubisco catalyzed reaction. Chemical Physics Letters, 1997, 278, 291-296.	1.2	17
287	Theory of non-local (pair site) reactivity from model static-density response functions. Theoretical Chemistry Accounts, 1998, 99, 183-191.	0.5	17
288	Experimental and theoretical study on the piezoelectric behavior of barium doped PZT. Journal of Materials Science, 1999, 34, 3659-3667.	1.7	17

#	Article	IF	Citations
289	A DFT Study of the Molecular Mechanisms of the Dielsâ˜Alder Reaction between Cyclopentadiene and 3-Phenyl-1-(2-pyridyl)-2-propen-1-one â˜ Role of the Zn2+ Lewis Acid Catalyst and Water Solvent. European Journal of Organic Chemistry, 2002, 2002, 2557.	1.2	17
290	Calculation of binding energy using BLYP/MM for the HIV-1 integrase complexed with the S-1360 and two analogues. Bioorganic and Medicinal Chemistry, 2007, 15, 3818-3824.	1.4	17
291	A DFT study of methanol dissociation on isolated vanadate groups. Catalysis Today, 2008, 139, 214-220.	2.2	17
292	Structural, electronic and optical properties of Fe(III) complex with pyridine-2,6-dicarboxylic acid: A combined experimental and theoretical study. Inorganica Chimica Acta, 2014, 416, 200-206.	1.2	17
293	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
294	Laser-induced formation of bismuth nanoparticles. Physical Chemistry Chemical Physics, 2018, 20, 13693-13696.	1.3	17
295	Computational procedure to an accurate DFT simulation to solid state systems. Computational Materials Science, 2019, 170, 109176.	1.4	17
296	Theoretical study of cluster models and molecular hydrogen interaction with SnO2 [110] surface. Computational and Theoretical Chemistry, 1995, 335, 167-174.	1.5	16
297	Piezoelectric behaviour of PZT doped with calcium: a combined experimental and theoretical study. Journal of Materials Science, 1997, 32, 2381-2386.	1.7	16
298	A quantum-chemical study of transition structures for enolization and oxygenation steps catalyzed by rubisco: on the role of magnesium and carbamylated Lys-201 in opening oxygen capture channel. Chemical Physics Letters, 2000, 323, 29-34.	1.2	16
299	Lewis Acid Mediated Domino Reaction between 2-Cyclohexenone and Methyl Azide - A DFT Study. European Journal of Organic Chemistry, 2005, 2005, 4705-4709.	1.2	16
300	Understanding the chemical reactivity of phenylhalocarbene systems: an analysis based on the spin-polarized density functional theory. Theoretical Chemistry Accounts, 2007, 118, 325-335.	0.5	16
301	Theoretical Study on the Reaction Mechanism of VO₂⁺ with Propyne in Gas Phase. Journal of Physical Chemistry A, 2008, 112, 1808-1816.	1.1	16
302	Quantum mechanical modeling of excited electronic states and their relationship to cathodoluminescence of BaZrO3. Journal of Applied Physics, 2013, 114, .	1.1	16
303	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
304	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
305	Connecting Theory with Experiment to Understand the Sintering Processes of Ag Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 11310-11318.	1.5	16
306	Polymorphs of ZnV₂O₆ under Pressure: A First-Principle Investigation. Journal of Physical Chemistry C, 2019, 123, 3239-3253.	1.5	16

#	Article	IF	Citations
307	Zinc-substituted Ag2CrO4: A material with enhanced photocatalytic and biological activity. Journal of Alloys and Compounds, 2020, 835, 155315.	2.8	16
308	Graphene Nanoplatelets: In Vivo and In Vitro Toxicity, Cell Proliferative Activity, and Cell Gene Expression. Applied Sciences (Switzerland), 2022, 12, 720.	1.3	16
309	A theoretical analysis on the intramolecular proton transfer of Î±-alanine in an aqueous medium. Chemical Physics Letters, 1998, 294, 1-8.	1.2	15
310	A Theoretical Study of the Molecular Mechanism for the Carboxylation Chemistry in Rubisco. Journal of Physical Chemistry A, 1999, 103, 8725-8732.	1.1	15
311	Transition Structures ford-Ribulose-1,5-bisphosphate Carboxylase/Oxygenase-Catalyzed Oxygenation Chemistry:Â Role of Carbamylated Lysine in a Model Magnesium Coordination Sphere. Journal of Physical Chemistry A, 2001, 105, 4726-4736.	1.1	15
312	An AM1 theoretical study on the effect of Zn2+ Lewis acid catalysis on the mechanism of the cycloaddition between 3-phenyl-1-(2-pyridyl)-2-propen-1-one and cyclopentadiene. Tetrahedron, 2002, 58, 2695-2700.	1.0	15
313	Homofugality: A new reactivity index describing the leaving group ability in homolytic substitution reactions. Chemical Physics Letters, 2006, 424, 437-442.	1.2	15
314	Disclosing the electronic structure and optical properties of Ag₄V₂O₇crystals: experimental and theoretical insights. CrystEngComm, 2016, 18, 6483-6491.	1.3	15
315	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
316	PVC-SiO2-Ag composite as a powerful biocide and anti-SARS-CoV-2 material. Journal of Polymer Research, 2021, 28, 1.	1.2	15
317	A PM3 Quantum Chemical Study of the Pyruvate Reduction Mechanism Catalyzed by Lactate Dehydrogenase. Bioorganic Chemistry, 1993, 21, 260-274.	2.0	14
318	CO interaction with ZnO surfaces: an MNDO, AM1 and PM3 theoretical study with large cluster models. Computational and Theoretical Chemistry, 1996, 363, 249-256.	1.5	14
319	Unimolecular Decomposition of the Anionic Form ofN-Chloro-Î±-glycine. A Theoretical Study. The Journal of Physical Chemistry, 1996, 100, 3561-3568.	2.9	14
320	Theoretical Study of the Molecular Mechanism for the Oxygenation Chemistry in Rubisco. Journal of Physical Chemistry A, 1999, 103, 6009-6016.	1.1	14
321	Electronic mechanistic pattern for Câ€“C bond-breaking from transition structures in Rubisco's chemistry. Chemical Physics Letters, 2001, 340, 391-399.	1.2	14
322	Two state reactivity mechanism for the rearrangement of hydrogen peroxynitrite to nitric acid. Chemical Physics Letters, 2008, 457, 216-221.	1.2	14
323	Experimental and theoretical approach of nanocrystalline TiO2 with antifungal activity. Chemical Physics Letters, 2013, 577, 114-120.	1.2	14
324	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

#	Article	IF	Citations
325	Designing biocompatible and multicolor fluorescent hydroxyapatite nanoparticles for cell-imaging applications. Materials Today Chemistry, 2019, 14, 100211.	1.7	14
326	First principle investigation of the exposed surfaces and morphology of Î²-ZnMoO4. Journal of Applied Physics, 2019, 126, 235301.	1.1	14
327	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
328	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
329	Comparison of Several Semiempirical and ab Initio Methods for Transition State Structure Characterization. Addition of CO2 to CH3NHCONH2. The Journal of Physical Chemistry, 1994, 98, 3664-3668.	2.9	13
330	On a possible invariance of a transition structure to the effects produced by ancillary H-bonding molecules: Modeling the effects of Ser-48 in the hydride-transfer step of liver alcohol dehydrogenase. International Journal of Quantum Chemistry, 1996, 57, 245-257.	1.0	13
331	Inactivation of Ribulose-1,5-bisphosphate Carboxylase/Oxygenase during Catalysis. A Theoretical Study of Related Transition Structures. The Journal of Physical Chemistry, 1996, 100, 8543-8550.	2.9	13
332	Molecular mechanism for oxygenation pathway in Rubisco.. Chemical Physics Letters, 1998, 294, 87-94.	1.2	13
333	Conformational equilibrium of chorismate. A QM/MM theoretical study combining statistical simulations and geometry optimisations in gas phase and in aqueous solution. Computational and Theoretical Chemistry, 2003, 632, 197-206.	1.5	13
334	Composition Dependence of the Energy Barrier for Lithium Diffusion in Amorphous WO[sub 3]. Electrochemical and Solid-State Letters, 2005, 8, J21.	2.2	13
335	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
336	Increasing the photocatalytic and fungicide activities of Ag3PO4 microcrystals under visible-light irradiation. Ceramics International, 2021, 47, 22604-22614.	2.3	13
337	Calculation of the relative basicities of methylamines in solution. Chemical Physics Letters, 1990, 169, 297-300.	1.2	12
338	ZnO clusters models: AnAM1 andMNDO study. International Journal of Quantum Chemistry, 1993, 48, 643-653.	1.0	12
339	Ab initio and semiempirical MO studies using large cluster models of CO and H2 adsorption and dissociation on ZnO surfaces with the formation of ZnH and OH species. Computational and Theoretical Chemistry, 1997, 397, 147-157.	1.5	12
340	A density functional theory analysis of the gas and solution phase isomerization reactions of MCN, (M) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.5	12
341	Density functional theory study of the oxidation of methanol to formaldehyde on a hydrated vanadia cluster. Journal of Computational Chemistry, 2010, 31, 2493-2501.	1.5	12
342	N, P, and As Ylides and Aza- and Arsa-Wittig Reactions from Topological Analyses of Electron Density. Journal of Physical Chemistry A, 2011, 115, 8316-8326.	1.1	12

#	Article	IF	Citations
343	Toward an Understanding of the Hydrogenation Reaction of MO₂ Gas-Phase Clusters (M =) Tj ETQq1 1 0.784314 rgBT /O	1.1	12
344	Oxygen Atom Transfer Reactions from Mimoun Complexes to Sulfides and Sulfoxides. A Bonding Evolution Theory Analysis. Journal of Physical Chemistry A, 2014, 118, 6092-6103.	1.1	12
345	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
346	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
347	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
348	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
349	Quantum-chemical studies of the energy hypersurface for the Meyerâ€"Schuster rearrangement STO-3G calculation of minimum-energy paths. Intermolecular mechanism. Chemical Physics Letters, 1983, 94, 193-197.	1.2	11
350	A quantum chemical study of protonated intermediates in Rupe and Meyer-Schuster rearrangement mechanisms. Computational and Theoretical Chemistry, 1983, 105, 307-314.	1.5	11
351	Transition state structures for the molecular mechanism of lactate dehydrogenase enzyme. Journal of the Chemical Society Perkin Transactions II, 1995, , 1551-1558.	0.9	11
352	Enzyme catalysis: Transition structures and quantum dynamical aspects: Modeling rubisco's oxygenation and carboxylation mechanisms. International Journal of Quantum Chemistry, 2002, 88, 154-166.	1.0	11
353	A theoretical study on the thermal ring opening rearrangement of 1H-bicyclo[3.1.0]hexa-3,5-dien-2-one: a case of two state reactivity. Physical Chemistry Chemical Physics, 2009, 11, 7189.	1.3	11
354	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
355	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
356	A theoretical study of the intramolecular solvolytic mechanism of the Meyerâ€"Schuster reaction. MINDO/3 and CNDO/2 calculations of minimum energy paths. Computational and Theoretical Chemistry, 1983, 105, 49-54.	1.5	10
357	A theoretical study of the addition mechanism of carbon dioxide to methylamine. Modelling CO2â€"biotin fixation. Journal of the Chemical Society Perkin Transactions II, 1993, , 521-523.	0.9	10
358	Pseudopotential Periodic Hartree-Fock study of K8In11 and Rb8In11 Systems. The Journal of Physical Chemistry, 1995, 99, 12483-12487.	2.9	10
359	A PM3 theoretical study of the adsorption and dissociation of water on MgO surfaces. Computational and Theoretical Chemistry, 1998, 426, 199-205.	1.5	10
360	Transition-state structures for describing the enzyme-catalyzed mechanisms of rubisco. Theoretical Chemistry Accounts, 1999, 101, 234-240.	0.5	10

#	Article	IF	Citations
361	Theoretical analysis on TiO2(110)/V surface. International Journal of Quantum Chemistry, 2001, 85, 44-51.	1.0	10
362	The use of the generator coordinate method for designing basis set. Application to oxo-diperoxo molybdenum complexes. Computational and Theoretical Chemistry, 2002, 589-590, 251-264.	1.5	10
363	Exploring Two-State Reactivity Pathways in the Cycloaddition Reactions of Triplet Methylene. Journal of Physical Chemistry A, 2005, 109, 4178-4184.	1.1	10
364	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
365	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
366	Synthesis of Cuboctahedral CeO₂ Nanoclusters and Their Assembly into Cuboid Nanoparticles by Oriented Attachment. ChemNanoMat, 2017, 3, 228-232.	1.5	10
367	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
368	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
369	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
370	Structure, Photoluminescence Emissions, and Photocatalytic Activity of Ag₂SeO₃: A Joint Experimental and Theoretical Investigation. Inorganic Chemistry, 2021, 60, 5937-5954.	1.9	10
371	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
372	Garnet Crystal Structures. An ab Initio Perturbed Ion Study. The Journal of Physical Chemistry, 1995, 99, 6493-6501.	2.9	9
373	Theoretical study of substituent effects in the unimolecular decomposition of N-chloro-?-amino acid anions. Analysis of transition structure and molecular reaction mechanism. Journal of Physical Organic Chemistry, 1996, 9, 371-380.	0.9	9
374	A theoretical study on the decomposition mechanism of Î²-propiolactone and Î²-butyrolactone. Chemical Physics Letters, 1998, 288, 261-269.	1.2	9
375	The tandem Diels-Alder reaction between acetylenedicarboxyaldehyde and N,N'-dipyrrolylmethane. An ab initio study of the molecular mechanisms. Computational and Theoretical Chemistry, 1998, 426, 257-262.	1.5	9
376	A theoretical study of the unimolecular decomposition of N-chloro-Î±-amino acids in aqueous solution. Chemical Physics, 1998, 229, 125-136.	0.9	9
377	Transition State Structures and Intermediates Modeling Carboxylation Reactions Catalyzed by Rubisco. A Quantum Chemical Study of the Role of Magnesium and Its Coordination Sphere. Journal of Physical Chemistry A, 2001, 105, 9243-9251.	1.1	9
378	Towards a Rational Design of Antibody Catalysts through Computational Chemistry. Angewandte Chemie - International Edition, 2005, 44, 904-909.	7.2	9

#	Article	IF	Citations
379	Theoretical Study of Catalytic Efficiency of a Dielsâ€“Alderase Catalytic Antibody: An Indirect Effect Produced During the Maturation Process. Chemistry - A European Journal, 2008, 14, 596-602.	1.7	9
380	Synthesis and Molecular and Electronic Structures of a Series of Mo₃CoSe₄ Cluster Complexes with Three Different Metal Electron Populations. Inorganic Chemistry, 2008, 47, 3661-3668.	1.9	9
381	Prediction of dopant atom distribution on nanocrystals using thermodynamic arguments. Physical Chemistry Chemical Physics, 2014, 16, 1089-1094.	1.3	9
382	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
383	Electron beam irradiation for the formation of thick Ag film on Ag₃PO₄. RSC Advances, 2020, 10, 21745-21753.	1.7	9
384	Femtosecond-laser-irradiation-induced structural organization and crystallinity of Bi2WO6. Scientific Reports, 2020, 10, 4613.	1.6	9
385	Connecting morphology and photoluminescence emissions in Î²-Ag2MoO4 microcrystals. Ceramics International, 2022, 48, 3740-3750.	2.3	9
386	Tailoring Bi2MoO6 by Eu3+ incorporation for enhanced photoluminescence emissions. Journal of Luminescence, 2022, 243, 118675.	1.5	9
387	Bridging experiment and theory: Morphology, optical, electronic, and magnetic properties of MnWO4. Applied Surface Science, 2022, 600, 154081.	3.1	9
388	Theoretical rotational constants of MeCnN species. Chemical Physics Letters, 1990, 166, 54-56.	1.2	8
389	Theoretical study of stationary structures of acetamidine unimolecular decomposition. Chemical Physics Letters, 1990, 169, 509-512.	1.2	8
390	Local Relaxation Effects in the Crystal Structure of Vanadium-Doped Zircon. An ab Initio Perturbed Ion Calculation. The Journal of Physical Chemistry, 1994, 98, 7741-7744.	2.9	8
391	Transition structures for hydride transfer reactions in vacuo and their role in enzyme catalysis. Computational and Theoretical Chemistry, 1996, 371, 299-312.	1.5	8
392	The tandem Diels-Alder reaction of dimethyl acetylenedicarboxylate to bicyclopentadiene. A theoretical study of the molecular mechanisms. Tetrahedron Letters, 1996, 37, 7573-7576.	0.7	8
393	Towards an understanding of the molecular mechanism of the unimolecular decomposition of the N-chloro-Î±-amino acids on the ground and excited states surfaces in aqueous medium. Chemical Physics Letters, 1998, 283, 294-300.	1.2	8
394	Theoretical Study on the Molecular Mechanism of the Domino Cycloadditions between Dimethyl Acetylenedicarboxylate and Naphthaleno- and Anthracenofuranophane. Journal of Organic Chemistry, 1999, 64, 3026-3033.	1.7	8
395	A theoretical study on the molecular mechanism for the normal Reimerâ€“Tiemann reaction. Chemical Physics Letters, 2000, 318, 270-275.	1.2	8
396	Theoretical QM/MM studies of enzymatic pericyclic reactions. Interdisciplinary Sciences, Computational Life Sciences, 2010, 2, 115-131.	2.2	8

#	Article	IF	Citations
397	Molecular mechanism of chorismate mutase activity of promiscuos MbtI. Theoretical Chemistry Accounts, 2011, 128, 601-607.	0.5	8
398	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
399	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
400	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
401	Structure, optical properties, and photocatalytic activity of Î±-Ag2W0.75Mo0.25O4. Materials Research Bulletin, 2020, 132, 111011.	2.7	8
402	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
403	An ab initio perturbed ion study of bulk ceria. Chemical Physics Letters, 1994, 221, 249-254.	1.2	7
404	A Joint Experimental and Theoretical Study on the Mechanisms of Methyl 2-Hydroxypropionate and Methyl 2-Hydroxyisobutyrate Decomposition in the Gas Phase. Journal of Physical Chemistry A, 2004, 108, 996-1007.	1.1	7
405	Photoluminescence in quasi-amorphous Pb0.8X0.2Zr0.53Ti0.47O3 (X=Ca, Sr and Ba) powders: An optical and structural study. Chemical Physics Letters, 2009, 475, 96-100.	1.2	7
406	A joint computational and experimental study of a novel dioxomolybdenum(VI) complex bearing chiral N,N-dimethyllactamide ligand. Inorganica Chimica Acta, 2011, 375, 41-46.	1.2	7
407	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
408	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
409	Interface matters: Design of an efficient Î±-Ag2WO4/Ag3PO4 photocatalyst. Materials Chemistry and Physics, 2022, 280, 125710.	2.0	7
410	Inactivation of SARS-CoV-2 by a chitosan/Î±-Ag2WO4 composite generated by femtosecond laser irradiation. Scientific Reports, 2022, 12, 8118.	1.6	7
411	Catalytic role of copper(I) ion on the propargylic transposition. A theoretical study. The Journal of Physical Chemistry, 1985, 89, 4769-4773.	2.9	6
412	Electronic aspects of the hydride transfer mechanism. III. Ab-initio analytical gradient studies of the cyclopropenyl-cation/LiH with 4-31G and 3-21+G basis sets.. Computational and Theoretical Chemistry, 1988, 166, 421-430.	1.5	6
413	A comparative QCISD(T), DFT and MCSCF study of the unimolecular, decomposition of the N-chloro-Î±-glycine anion in gas phase. Theoretica Chimica Acta, 1996, 94, 247-256.	0.9	6
414	A quantum electronic theory of chemical processes?The inverted energy profile case: CH3+ + H2 reaction. International Journal of Quantum Chemistry, 1997, 63, 373-391.	1.0	6

#	Article	IF	Citations
415	PM3 study of the domino reaction of nitroalkenes with silyl enol ethers. Journal of Physical Organic Chemistry, 1999, 12, 24-30.	0.9	6
416	A joint theoretical and kinetic investigation on the fragmentation of (N-halo)-2-amino cycloalkanecarboxylates. Chemical Physics, 2002, 280, 1-14.	0.9	6
417	A theoretical study on the mechanism of the base-promoted decomposition of N-chloro,N-methylethanolamine. Organic and Biomolecular Chemistry, 2009, 7, 1807.	1.5	6
418	A DFT Study of the Reactivity Indexes of Ionic [4 + 2+] Diels-Alder Cycloaddition to Nitrilium and Immonium Ions. Letters in Organic Chemistry, 2011, 8, 104-107.	0.2	6
419	Structural and optical properties of ZnS/MgNb2O6 heterostructures. Superlattices and Microstructures, 2015, 79, 180-192.	1.4	6
420	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
421	A scalable electron beam irradiation platform applied for allotropic carbon transformation. Carbon, 2021, 174, 567-580.	5.4	6
422	A theoretical and experimental investigation of hetero- vs. homo-connectivity in barium silicates. American Mineralogist, 2022, 107, 716-728.	0.9	6
423	Photoluminescence emissions of Ca1â^'WO4:xEu3+: Bridging between experiment and DFT calculations. Journal of Rare Earths, 2022, 40, 1527-1534.	2.5	6
424	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
425	An ab initio study of the unimolecular decomposition mechanism of formamidine. 4-31G Characterization of potential energy hypersurface. International Journal of Quantum Chemistry, 1991, 40, 127-137.	1.0	5
426	Quantum Chemical Studies of Pyrroloquinoline Quinone: PM3 Pathways for Methanol Oxidation. Bioorganic Chemistry, 1994, 22, 58-71.	2.0	5
427	Periodic Hartree-Fock calculation of the A1g (Tz) and Eg (Tx, Ty) phonon modes in ice VIII. Journal of Molecular Structure, 1997, 436-437, 443-449.	1.8	5
428	A PM3 semiempirical study of the molecular mechanism for the Favorskii rearrangement of the Î±-chlorocyclobutanone. Computational and Theoretical Chemistry, 1998, 426, 299-306.	1.5	5
429	A PM3 study of the molecular mechanism for the cycloaddition between cyclopentadiene and protonated pyridine-imine derivatives. Computational and Theoretical Chemistry, 2001, 544, 79-90.	1.5	5
430	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.	1.2	5
431	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
432	Towards a white-emitting phosphor Ca10V6O25 based material. Journal of Luminescence, 2020, 220, 116990.	1.5	5

#	Article	IF	Citations
433	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
434	Behavior of Bi2S3 under ultrasound irradiation for Rhodamine B dye degradation. Chemical Physics Letters, 2021, 785, 139123.	1.2	5
435	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
436	Linear bending in propynyl cation, allene, and propyne systems: do they have flexible structures? an ab initio 4 â€“ 31 + G molecular orbital study. Journal of the Chemical Society Perkin Transactions II, 1985, , 363-366.	0.9	4
437	Theoretical studies of Î±-acetylenic alcohols rearrangement mechanism: Ab initio calculations of the unimolecular rate limiting step. Computational and Theoretical Chemistry, 1986, 138, 171-177.	1.5	4
438	V4+ doping into SiO2, ZrO2 and ZrSiO4 structures. Anab initio perturbed ion study. International Journal of Quantum Chemistry, 1993, 48, 175-186.	1.0	4
439	An Ab initio perturbed ion study of pyrope garnet structure. Journal of Physics and Chemistry of Solids, 1995, 56, 901-906.	1.9	4
440	A semiempirical study on the ring-opening process for the cyclopropanone, 2,2-dimethylcyclopropanone,trans-2,3-di-tert-butylcyclopropanone, and spiro(bicyclo[2.2.1]heptane-2.1?-cyclopropan)-2?-one systems in solution. International Journal of Quantum Chemistry, 1997, 65, 729-738.	1.0	4
441	Designing a Transition State Analogue for the Disfavored Intramolecular Michael Addition of 2-(2-Hydroxyethyl)acrylate Esters. Journal of Organic Chemistry, 1999, 64, 9164-9169.	1.7	4
442	Alternative pathways for the C2â€“C3 bond cleavage and C2 configuration inversion processes for the Rubisco-catalyzed carboxylation sequence. Chemical Physics Letters, 2000, 318, 361-369.	1.2	4
443	A Combined Experimental and Theoretical Study of the Homogeneous, Unimolecular Decomposition Kinetics of 3-Chloropivalic Acid in the Gas Phase. Journal of Physical Chemistry A, 2001, 105, 1869-1875.	1.1	4
444	Understanding the mechanism of base-assisted decomposition of (N-halo),N-alkylalcoholamines. Organic and Biomolecular Chemistry, 2003, 1, 4323-4328.	1.5	4
445	Density functional study of the Hoffmann elimination of (N-Cl),N-methylethanolamine in gas phase and in aqueous solution. Chemical Physics Letters, 2006, 429, 425-429.	1.2	4
446	Proton transport catalysis in intramolecular rearrangements: A density functional theory study. Chemical Physics Letters, 2008, 464, 271-275.	1.2	4
447	Photoluminescence Properties of Nanocrystals. Journal of Nanomaterials, 2012, 2012, 1-2.	1.5	4
448	Evidence for the formation of metallic In after laser irradiation of InP. Journal of Applied Physics, 2019, 126, .	1.1	4
449	Deciphering the Molecular Mechanism of Intramolecular Reactions from the Perspective of Bonding Evolution Theory. Physchem, 2022, 2, 207-223.	0.5	4
450	Simulation of ionic crystals: calculation of Madelung potentials for stabilized zirconia. Journal of Materials Science, 1995, 30, 4852-4856.	1.7	3

#	Article	IF	Citations
451	MgAl2O4 spinel crystal structure. An ab initio perturbed ion study. International Journal of Quantum Chemistry, 1995, 56, 685-694.	1.0	3
452	An ab Initio Perturbed Ion Study of the BaLiF3 and BaLiH3 Inverted Perovskite Structures. The Journal of Physical Chemistry, 1995, 99, 8082-8090.	2.9	3
453	Theoretical characterization of transition structure for the enzyme-catalyzed reaction at the active center of lactate dehydrogenase. Geometry and transition vector dependence upon computing method and model system. Journal of Physical Organic Chemistry, 1996, 9, 498-506.	0.9	3
454	Understanding the mechanism of the addition of organomagnesium reagents to 2-hydroxypropanal: An ab initio molecular orbital analysis. International Journal of Quantum Chemistry, 1997, 65, 719-728.	1.0	3
455	A theoretical study of the addition of CH3MgCl to chiral Î±-alkoxy carbonyl compounds. Computational and Theoretical Chemistry, 1998, 426, 263-275.	1.5	3
456	Theoretical investigation of the abnormal Reimer-Tiemann reaction. Journal of Physical Organic Chemistry, 1998, 11, 670-677.	0.9	3
457	Author Index to Volumes 271â€“280. Chemical Physics, 2002, 280, 1-26.	0.9	3
458	Towards a Rational Design of Antibody Catalysts through Computational Chemistry. Angewandte Chemie, 2005, 117, 926-931.	1.6	3
459	Stereoselectivity Behavior of the AZ28 Antibody Catalyzed Oxy-Cope Rearrangementâ€. Journal of Physical Chemistry A, 2006, 110, 726-730.	1.1	3
460	Combined ¹³C NMR and DFT/GIAO studies of the polyketides Aurasperone A and Fonsecinone A. International Journal of Quantum Chemistry, 2008, 108, 2408-2416.	1.0	3
461	New insight into the electronic structure of iron(IV)â€oxo porphyrin compound I. A quantum chemical topological analysis. Journal of Computational Chemistry, 2013, 34, 780-789.	1.5	3
462	Towards an Understanding on the Role of Precursor in the Synthesis of ZnS Nanostructures. Current Physical Chemistry, 2013, 3, 378-385.	0.1	3
463	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
464	Formation of Metallic Ag on AgBr by Femtosecond Laser Irradiation. Physchem, 2022, 2, 179-190.	0.5	3
465	Theoretical study of lattice stability and selective doping effects of V4+ and Tb4+ in the ZrGeO4 lattice. Chemical Physics Letters, 1995, 236, 521-531.	1.2	2
466	Ionic structures as intercalation compound host lattices. An ab initio perturbed ion study on lattice stretching. Computational and Theoretical Chemistry, 1995, 330, 313-317.	1.5	2
467	Ab initio perturbed ion calculations on Ni2+Â·KZnF3 and Ni2+ Â·KMgF3. A structural study. Computational and Theoretical Chemistry, 1995, 330, 319-323.	1.5	2
468	Hydrogen bonding and dissociation effects on the gas phase proton transfer reactions of ozone. Theoretical Chemistry Accounts, 1998, 99, 60-63.	0.5	2

#	Article	IF	Citations
469	Theoretical study of the molecular mechanism of the domino pathways for squarate ester sequential reactions. Journal of Physical Organic Chemistry, 1999, 12, 61-68.	0.9	2
470	Stability of MgAl 2 O 4 Under High-Pressure Conditions. High Pressure Research, 2002, 22, 447-450.	0.4	2
471	Bridging Structure and Real-Space Topology: Understanding Complex Molecules and Solid-State Materials. , 2017, , 427-454.		2
472	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
473	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
474	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
475	Unveiling the Ag-Bi miscibility at the atomic level: A theoretical insight. Computational Materials Science, 2021, 197, 110612.	1.4	2
476	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
477	Quantum Chemical Topology Approach for Dissecting Chemical Structure and Reactivity. Challenges and Advances in Computational Chemistry and Physics, 2016, , 257-294.	0.6	2
478	MO studies of the nature of the bifurcated hydrogen bond. Rotational barriers in cyclohexanol and 1,3-dioxan-5-ol. Chemical Physics Letters, 1984, 109, 468-470.	1.2	1
479	Theoretical studies of substituent effects on stationary structures of amidine decomposition. Journal of the Chemical Society Perkin Transactions II, 1991, , 539-542.	0.9	1
480	Transition structure for hydride transfer from cyclopropene to azirinium cation. Computational and Theoretical Chemistry, 1996, 363, 257-261.	1.5	1
481	Metallic behavior in STO/LAO heterostructures with non-uniformly atomic interfaces. Materials Today Communications, 2020, 24, 101339.	0.9	1
482	Quantum Theory of Solvent Effects and Chemical Reactions. , 2002, , 283-361.		1
483	GENERALIZED DIABATIC STUDY OF ETHYLENE â€œISOMERISMâ€œ. , 2006, , 177-196.		1
484	Hybrid QM/MM Studies on Chemical Reactivity. ChemInform, 2003, 34, no.	0.1	0
485	Theoretical Insights in Enzyme Catalysis. ChemInform, 2004, 35, no.	0.1	0
486	A Theoretical Study on the Gas Phase Reactions of the Anions NbO3-, NbO5-, and NbO2(OH)2- with H2O and O2. ChemInform, 2005, 36, no.	0.1	0

#	Article	IF	Citations
487	DFT Study of Oxygen Adsorption on Modified Nanostructured Gold Pyramids.. ChemInform, 2005, 36, no.	0.1	0
488	Topological Analysis of the Bonds in Incomplete Cuboidal [Mo₃S₄] Clusters.. ChemInform, 2002, 33, 2-2.	0.1	0
489	A Thermodynamic Approach to Predict Dopant Atoms Segregation on Nanocrystals. Microscopy and Microanalysis, 2011, 17, 1458-1459.	0.2	0
490	Chemical Bonding under Pressure. , 2015, , 131-157.		0