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List of Publications by Citations

481 papers	13,505 citations	61 h-index	81 g-index
504 ext. papers	14,720 ext. citations	4.3 avg, IF	6.39 L-index

#	Paper	IF	Citations
481	Crystal growth in colloidal tin oxide nanocrystals induced by coalescence at room temperature. *Applied Physics Letters*, **2003**, 83, 1566-1568	3.4	237
480	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	8.4	157
479	Morphology and Blue Photoluminescence Emission of PbMoO4 Processed in Conventional Hydrothermal. *Journal of Physical Chemistry C*, **2009**, 113, 5812-5822	3.8	156
478	Understanding reaction mechanisms in organic chemistry from catastrophe theory applied to the electron localization function topology. *Journal of Physical Chemistry A*, **2008**, 112, 7128-36	2.8	147
477	The Joint Use of Catastrophe Theory and Electron Localization Function to Characterize Molecular Mechanisms. A Density Functional Study of the Diels□Alder Reaction between Ethylene and 1,3-Butadiene. *Journal of Physical Chemistry A*, **2003**, 107, 6014-6024	2.8	134
476	Electronic structure and optical properties of BaMoO4 powders. *Current Applied Physics*, **2010**, 10, 614-624	2.4	130
475	An Aromaticity Scale Based on the Topological Analysis of the Electron Localization Function Including □and □Contributions. *Journal of Chemical Theory and Computation*, **2005**, 1, 83-6	6.4	130
474	Theoretical insights in enzyme catalysis. *Chemical Society Reviews*, **2004**, 33, 98-107	58.5	129
473	Influence of Reactant Polarity on the Course of the Inverse-Electron-Demand Diels□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	4.2	122
472	New findings on the Diels-Alder reactions. An analysis based on the bonding evolution theory. *Journal of Physical Chemistry A*, **2006**, 110, 13939-47	2.8	114
471	Hierarchical Assembly of CaMoO4 Nano-Octahedrons and Their Photoluminescence Properties. *Journal of Physical Chemistry C*, **2011**, 115, 5207-5219	3.8	113
470	Toward an Understanding of the Growth of Ag Filaments on □Ag2WO4 and Their Photoluminescent Properties: A Combined Experimental and Theoretical Study. *Journal of Physical Chemistry C*, **2014**, 118, 1229-1239	3.8	111
469	Facet-dependent photocatalytic and antibacterial properties of □Ag2WO4 crystals: combining experimental data and theoretical insights. *Catalysis Science and Technology*, **2015**, 5, 4091-4107	5.5	110
468	Static simulation of bulk and selected surfaces of anatase TiO2. *Surface Science*, **2001**, 490, 116-124	1.8	106
467	Thermodynamic argument about SnO2 nanoribbon growth. *Applied Physics Letters*, **2003**, 83, 635-637	3.4	105
466	Density functional theory study of the brookite surfaces and phase transitions between natural titania polymorphs. *Journal of Physical Chemistry B*, **2006**, 110, 23417-23	3.4	103
465	A Systematic Density Functional Theory Study of VxOy+ and VxOY (X = 2□4, Y = 2□10) Systems. *Journal of Physical Chemistry A*, **2001**, 105, 9760-9775	2.8	102

464	Direct in situ observation of the electron-driven synthesis of Ag filaments on Ag2WO4 crystals. *Scientific Reports*, **2013**, 3, 1676	4.9	95
463	Density functional theory calculation of the electronic structure of Ba0.5Sr0.5TiO3: Photoluminescent properties and structural disorder. *Physical Review B*, **2004**, 69,	3.3	94
462	Room-temperature photoluminescence of BaTiO3: Joint experimental and theoretical study. *Physical Review B*, **2005**, 71,	3.3	93
461	Experimental and Theoretical Study on the Structure, Optical Properties, and Growth of Metallic Silver Nanostructures in Ag3PO4. *Journal of Physical Chemistry C*, **2015**, 119, 6293-6306	3.8	92
460	A novel ozone gas sensor based on one-dimensional (1D) Ag2WO4 nanostructures. *Nanoscale*, **2014**, 6, 4058-62	7.7	92
459	Efficient microwave-assisted hydrothermal synthesis of CuO sea urchin-like architectures via a mesoscale self-assembly. *CrystEngComm*, **2010**, 12, 1696	3.3	92
458	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	1.8	92
457	Potentiated electron transference in Ag2WO4 microcrystals with Ag nanofilaments as microbial agent. *Journal of Physical Chemistry A*, **2014**, 118, 5769-78	2.8	91
456	A Theoretical Study on the Relationship between Nucleophilicity and Ionization Potentials in Solution Phase. *Journal of Physical Chemistry A*, **2003**, 107, 5588-5593	2.8	87
455	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, 5165-72	4.8	86
454	A hybrid potential reaction path and free energy study of the chorismate mutase reaction. *Journal of the American Chemical Society*, **2001**, 123, 1709-12	16.4	84
453	Zinc blende versus wurtzite ZnS nanoparticles: control of the phase and optical properties by tetrabutylammonium hydroxide. *Physical Chemistry Chemical Physics*, **2014**, 16, 20127-37	3.6	82
452	Enhancing reactivity of carbonyl compounds via hydrogen-bond formation. A DFT study of the hetero-Diels-Alder reaction between butadiene derivative and acetone in chloroform. *Journal of Organic Chemistry*, **2003**, 68, 8662-8	4.2	81
451	Synthesis of wurtzite ZnS nanoparticles using the microwave assisted solvothermal method. *Journal of Alloys and Compounds*, **2013**, 556, 153-159	5.7	78
450	ZnWO nanocrystals: synthesis, morphology, photoluminescence and photocatalytic properties. *Physical Chemistry Chemical Physics*, **2018**, 20, 1923-1937	3.6	77
449	Theoretical modeling of enzyme catalytic power: analysis of "cratic" and electrostatic factors in catechol O-methyltransferase. *Journal of the American Chemical Society*, **2003**, 125, 7726-37	16.4	77
448	Structural and electronic analysis of the atomic scale nucleation of Ag on Ag2WO4 induced by electron irradiation. *Scientific Reports*, **2014**, 4, 5391	4.9	76
447	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	3.5	76

446	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, 12386-93	3.6	74
445	Presence of excited electronic state in CaWO4 crystals provoked by a tetrahedral distortion: An experimental and theoretical investigation. *Journal of Applied Physics*, **2011**, 110, 043501	2.5	74
444	A relationship between structural and electronic order-disorder effects and optical properties in crystalline TiO2 nanomaterials. *Dalton Transactions*, **2015**, 44, 3159-75	4.3	73
443	Silver Molybdate and Silver Tungstate Nanocomposites with Enhanced Photoluminescence. *Nanomaterials and Nanotechnology*, **2014**, 4, 22	2.9	72
442	Describing the Molecular Mechanism of Organic Reactions by Using Topological Analysis of Electronic Localization Function. *Current Organic Chemistry*, **2011**, 15, 3566-3575	1.7	71
441	Nine questions on energy decomposition analysis. *Journal of Computational Chemistry*, **2019**, 40, 2248-2283	3.3	70
440	Effects of surface stability on the morphological transformation of metals and metal oxides as investigated by first-principles calculations. *Nanotechnology*, **2015**, 26, 405703	3.4	70
439	A simple protocol to help calculate saddle points. Transition-state structures for the Meyer?Schuster reaction in non-aqueous media: An ab initio MO study. *Chemical Physics Letters*, **1984**, 109, 471-477	2.5	70
438	Toward Understanding the Photocatalytic Activity of PbMoO4 Powders with Predominant (111), (100), (011), and (110) Facets. A Combined Experimental and Theoretical Study. *Journal of Physical Chemistry C*, **2013**, 117, 21382-21395	3.8	69
437	Structure and Bonding of Chlorine Oxides and Peroxides:?ClOx, ClOx-(x= 1?4), and Cl2Ox(x= 1?3). *Journal of Physical Chemistry A*, **1999**, 103, 3078-3088	2.8	69
436	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	16.4	69
435	Theoretical Study on the Molecular Mechanism for the Reaction of VO2+ with C2H4. *Journal of Physical Chemistry A*, **2003**, 107, 3107-3120	2.8	68
434	A Joint Experimental and Theoretical Study on the Nanomorphology of CaWO4 Crystals. *Journal of Physical Chemistry C*, **2011**, 115, 20113-20119	3.8	66
433	Electronic and structural properties of SnxTi1?xO2 solid solutions: a periodic DFT study. *Catalysis Today*, **2003**, 85, 145-152	5.3	66
432	A theoretical study on the structure, energetics and bonding of VOx+ and VOx (x=1?4) systems. *Chemical Physics Letters*, **2001**, 333, 493-503	2.5	66
431	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	16.4	66
430	A combined theoretical and experimental study of electronic structure and optical properties of ?ZnMoO4 microcrystals. *Polyhedron*, **2013**, 54, 13-25	2.7	65
429	Characterization of the high-pressure structures and phase transformations in SnO2. A density functional theory study. *Journal of Physical Chemistry B*, **2007**, 111, 6479-85	3.4	65

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427	An efficient microwave-assisted hydrothermal synthesis of BaZrO3 microcrystals: growth mechanism and photoluminescence emissions. *CrystEngComm*, **2010**, 12, 3612	3.3	64
426	An improved method for preparation of SrTiO3 nanoparticles. *Materials Chemistry and Physics*, **2011**, 125, 168-173	4.4	63
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424	The hierarchy of localization basins: a tool for the understanding of chemical bonding exemplified by the analysis of the VOx and VOx+ (x=1,2) systems. *Theoretical Chemistry Accounts*, **2001**, 105, 299-308	1.9	63
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421	DFT Study of the Reaction between VO2+ and C2H6. *Organometallics*, **2004**, 23, 730-739	3.8	61
420	Unraveling reaction mechanisms by means of Quantum Chemical Topology Analysis. *International Journal of Quantum Chemistry*, **2014**, 114, 1239-1252	2.1	60
419	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	16.4	60
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417	On the photoluminescence behavior of samarium-doped strontium titanate nanostructures under UV light. A structural and electronic understanding. *Physical Chemistry Chemical Physics*, **2010**, 12, 7566-79	3.6	58
416	Structural refinement, growth mechanism, infrared/Raman spectroscopies and photoluminescence properties of PbMoO4 crystals. *Polyhedron*, **2013**, 50, 532-545	2.7	57
415	Towards understanding of magnetic interactions within a series of tetrathiafulvalene-pi conjugated-verdazyl diradical cation system: a density functional theory study. *Physical Chemistry Chemical Physics*, **2008**, 10, 857-64	3.6	57
414	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, 8970-8	2.8	57
413	Origin of photoluminescence in SrTiO3: a combined experimental and theoretical study. *Journal of Solid State Chemistry*, **2004**, 177, 3879-3885	3.3	57
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411	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, 8943-52	2.8	55

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408	Chemical structure and reactivity by means of quantum chemical topology analysis. *Computational and Theoretical Chemistry*, **2015**, 1053, 17-30	2	53
407	The interplay between morphology and photocatalytic activity in ZnO and N-doped ZnO crystals. *Materials and Design*, **2017**, 120, 363-375	8.1	52
406	Photoluminescence and Photocatalytic Properties of Ag PO Microcrystals: An Experimental and Theoretical Investigation. *ChemPlusChem*, **2016**, 81, 202-212	2.8	52
405	Elucidating the real-time Ag nanoparticle growth on Ag2WO4 during electron beam irradiation: experimental evidence and theoretical insights. *Physical Chemistry Chemical Physics*, **2015**, 17, 5352-9	3.6	52
404	Identifying and rationalizing the morphological, structural, and optical properties of [Formula: see text]-AgMoO microcrystals, and the formation process of Ag nanoparticles on their surfaces: combining experimental data and first-principles calculations. *Science and Technology of Advanced Materials*, **2015**, 16, 065002	7.1	52
403	Quantum Mechanics Insight into the Microwave Nucleation of SrTiO3 Nanospheres. *Journal of Physical Chemistry C*, **2012**, 116, 24792-24808	3.8	52
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401	Preorganization and reorganization as related factors in enzyme catalysis: the chorismate mutase case. *Chemistry - A European Journal*, **2003**, 9, 984-91	4.8	52
400	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, 3687-93	2.8	50
399	Theoretical Study of the Gas Phase Decomposition of Glycolic, Lactic, and 2-Hydroxyisobutyric Acids. *Journal of the American Chemical Society*, **1997**, 119, 6415-6422	16.4	49
398	Spin-Philicity and Spin-Donicity as Auxiliary Concepts To Quantify Spin-Catalysis Phenomena. *Journal of Physical Chemistry A*, **2002**, 106, 5353-5357	2.8	48
397	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, 8183-95	5.8	48
396	Lithium insertion and mobility in the TiO2-anatase/titanate structure: A periodic DFT study. *Journal of Electroanalytical Chemistry*, **2005**, 581, 216-223	4.1	47
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394	Mechanism of Antibacterial Activity via Morphology Change of AgVO: Theoretical and Experimental Insights. *ACS Applied Materials & Interfaces*, **2017**, 9, 11472-11481	9.5	46
393	A 3D platform for the morphology modulation of materials: first principles calculations on the thermodynamic stability and surface structure of metal oxides: Co3O4,Fe2O3, and In2O3. *Modelling and Simulation in Materials Science and Engineering*, **2016**, 24, 025007	2	46

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389	Surfactant-Mediated Morphology and Photocatalytic Activity of Ag2WO4 Material. *Journal of Physical Chemistry C*, **2018**, 122, 8667-8679	3.8	45
388	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	2.8	44
387	Contribution of structural order-disorder to the green photoluminescence of PbWO4. *Physical Review B*, **2007**, 75,	3.3	44
386	Following the molecular mechanism for the NH3 + LiH -g 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, 1663-72	2.8	43
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384	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		43
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375	Insight into the Effects of Fe Addition on the Local Structure and Electronic Properties of SrTiO3. *Journal of Physical Chemistry C*, **2014**, 118, 4930-4940	3.8	40

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366	On the nature of the transition state in catechol O-methyltransferase. A complementary study based on molecular dynamics and potential energy surface explorations. *Journal of the American Chemical Society*, **2005**, 127, 10648-55	16.4	39
365	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		39
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340	Microwave-hydrothermal synthesis of single-crystalline Co3O4 spinel nanocubes. *CrystEngComm*, **2013**, 15, 7443	3.3	33
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